

**Figure 1****Table 1.** Crystallographic data and refinement statistics

	Native data set
Wavelength (Å)	1.0526
Resolution range (Å) <sup>1</sup>	50.0-2.0 (2.07-2.0)
No. of observed reflections	164,206
No. of unique reflections	27,881
No. of reflections in R <sub>free</sub> set	828
Completeness (%)	99.2(99.4)
I/σ(I)	19.6(1.4)
(R <sub>merge</sub> ) (%) <sup>2</sup>	3.9(20.9)
R <sub>cryst</sub> /R <sub>free</sub> (%) <sup>3</sup>	21.8/23.8
No. of refined non-hydrogen atoms <sup>4</sup>	
protein	2248
water	265
Average B-factor (all atoms, Å <sup>2</sup> )	60
Wilson B-factor (Å <sup>2</sup> )	45
R.m.s. Δ bond lengths/angles <sup>5</sup>	0.0081/1.7
Residues in allowed regions (%) <sup>6</sup>	97%

<sup>1</sup>Values in parentheses are statistics for the highest resolution bin.

<sup>2</sup> $R_{\text{merge}}(I) = \sum_{hkl} |I_{hkl} - \langle I_{hkl} \rangle| / \sum_{hkl} I_{hkl}$ , where  $I_{hkl}$  is the measured intensity of the reflections with indices  $hkl$ .

<sup>3</sup> $R = \sum_{hkl} ||F_o| - |F_c|| / \sum |F_o|$ , where  $|F_o|$  and  $|F_c|$  are the observed and calculated structure factor amplitudes for reflection  $hkl$ , applied to the work (R<sub>cryst</sub>=97%) and test (R<sub>free</sub>=3%) sets, respectively.

<sup>4</sup>Residues -2, 239 and 240 were not located. Residues originating from the cloning site were given negative integers.

<sup>5</sup>Root mean squared deviations (rms Δ) in bond length and angles from ideal values.

<sup>6</sup>The Ramachandran plot was calculated according to Kleywegt and Jones, (1996).

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Figure 2 (Table 2 (page 1))

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HEADER      CELL ADHESION                                1QZ1
TITLE       CRYSTAL STRUCTURE OF THE IG 1-2-3 FRAGMENT OF NCAM
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: NEURAL CELL ADHESION MOLECULE 1, 140 KDA ISOFORM;
COMPND      3 CHAIN: A;
COMPND      4 FRAGMENT: IG MODULES 1-2-3;
COMPND      5 SYNONYM: N-CAM 140, NCAM-140;
COMPND      6 ENGINEERED: YES
SOURCE      MOL_ID: 1;
SOURCE      2 ORGANISM_SCIENTIFIC: RATTUS NORVEGICUS;
SOURCE      3 ORGANISM_COMMON: RAT;
SOURCE      4 GENE: NCAM1;
SOURCE      5 EXPRESSION_SYSTEM: PICHIA PASTORIS;
SOURCE      6 EXPRESSION_SYSTEM_COMMON: FUNGUS;
SOURCE      7 EXPRESSION_SYSTEM_STRAIN: GS-115;
SOURCE      8 EXPRESSION_SYSTEM_VECTOR_TYPE: PLASMID;
SOURCE      9 EXPRESSION_SYSTEM_PLASMID: PHIL-S1
KEYWDS      IG MODULES, CELL ADHESION, NCAM
EXPDTA      X-RAY DIFFRACTION
AUTHOR      V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICH, J.BREED,
AUTHOR      2 V.V.KISELYOV, F.M.POULSEN, I.LARSEN, W.WELTE, V.BEREZIN,
AUTHOR      3 E. BOCK, C.KASPER
JRNL        AUTH V.SOROKA, K.KOLKOVA, J.S.KASTRUP, K.DIEDERICH,
JRNL        AUTH 2 J.BREED, V.V. KISELYOV, F.M.POULSEN, I.LARSEN,
JRNL        AUTH 3 W.WELTE, V.BEREZIN, E. BOCK, C.KASPER
JRNL        TITL  STRUCTURE AND INTERACTIONS OF NCAM IG1-2-3 SUGGEST
JRNL        TITL 2 A NOVEL ZIPPER MECHANISM FOR HOMOPHILIC ADHESION
JRNL        REF   TO BE PUBLISHED
JRNL        REFN
REMARK      1
REMARK      1 REFERENCE 1
REMARK      1 AUTH C.KASPER, H.RASMUSSEN, J.S.KASTRUP, S.IKEMIZU,
REMARK      1 AUTH 2 E.Y.JONES, V.BEREZIN, E. BOCK, I.K.LARSEN
REMARK      1 TITL  STRUCTURAL BASIS OF CELL-CELL ADHESION BY NCAM
REMARK      1 REF   NAT.STRUCT.BIOL. V. 7 389 2000
REMARK      1 REFN  ASTM NSBIEW US ISSN 1072-8368
REMARK      1 REFERENCE 2
REMARK      1 AUTH C.KASPER, H.RASMUSSEN, V.BEREZIN, E. BOCK, I.K.LARSEN
REMARK      1 TITL  EXPRESSION, CRYSTALLIZATION AND PRELIMINARY X-RAY
REMARK      1 TITL 2 ANALYSIS OF THE TWO AMINO-TERMINAL IG DOMAINS OF
REMARK      1 TITL 3 THE NEURAL CELL ADHESION MOLECULE (NCAM)
REMARK      1 REF   ACTA CRYSTALLOGR., SECT.D V. 55 1598 1999
REMARK      1 REFN  ASTM ABCRE6 DK ISSN 0907-4449
REMARK      2
REMARK      2 RESOLUTION. 2.00 ANGSTROMS.
REMARK      3
REMARK      3 REFINEMENT.
REMARK      3 PROGRAM : CNS 1.0
REMARK      3 AUTHORS : BRUNGER, ADAMS, CLORE, DELANO, GROS, GROSSE-
REMARK      3 : KUNSTLEVE, JIANG, KUSZEWSKI, NILGES, PANNU,
REMARK      3 : READ, RICE, SIMONSON, WARREN
REMARK      3
REMARK      3 REFINEMENT TARGET : ENGH & HUBER
REMARK      3
REMARK      3 DATA USED IN REFINEMENT.
REMARK      3 RESOLUTION RANGE HIGH (ANGSTROMS) : 2.00
REMARK      3 RESOLUTION RANGE LOW (ANGSTROMS) : 48.64

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Figure 2 (Table 2 (page 2))

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REMARK 3 DATA CUTOFF (SIGMA(F)) : 0.000
REMARK 3 DATA CUTOFF HIGH (ABS(F)) : NULL
REMARK 3 DATA CUTOFF LOW (ABS(F)) : NULL
REMARK 3 COMPLETENESS (WORKING+TEST) (%) : 99.2
REMARK 3 NUMBER OF REFLECTIONS : 28289
REMARK 3
REMARK 3 FIT TO DATA USED IN REFINEMENT.
REMARK 3 CROSS-VALIDATION METHOD : THROUGHOUT
REMARK 3 FREE R VALUE TEST SET SELECTION : RANDOM
REMARK 3 R VALUE (WORKING SET) : 0.218
REMARK 3 FREE R VALUE : 0.238
REMARK 3 FREE R VALUE TEST SET SIZE (%) : NULL
REMARK 3 FREE R VALUE TEST SET COUNT : 828
REMARK 3 ESTIMATED ERROR OF FREE R VALUE : NULL
REMARK 3
REMARK 3 FIT IN THE HIGHEST RESOLUTION BIN.
REMARK 3 TOTAL NUMBER OF BINS USED : NULL
REMARK 3 BIN RESOLUTION RANGE HIGH (A) : 2.00
REMARK 3 BIN RESOLUTION RANGE LOW (A) : 2.13
REMARK 3 BIN COMPLETENESS (WORKING+TEST) (%) : 99.00
REMARK 3 REFLECTIONS IN BIN (WORKING SET) : NULL
REMARK 3 BIN R VALUE (WORKING SET) : 0.3730
REMARK 3 BIN FREE R VALUE : 0.4390
REMARK 3 BIN FREE R VALUE TEST SET SIZE (%) : NULL
REMARK 3 BIN FREE R VALUE TEST SET COUNT : 148
REMARK 3 ESTIMATED ERROR OF BIN FREE R VALUE : 0.036
REMARK 3
REMARK 3 NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK 3 PROTEIN ATOMS : 2247
REMARK 3 NUCLEIC ACID ATOMS : 0
REMARK 3 HETEROGEN ATOMS : 0
REMARK 3 SOLVENT ATOMS : 265
REMARK 3
REMARK 3 B VALUES.
REMARK 3 FROM WILSON PLOT (A**2) : 42.00
REMARK 3 MEAN B VALUE (OVERALL, A**2) : 60.60
REMARK 3 OVERALL ANISOTROPIC B VALUE.
REMARK 3 B11 (A**2) : 7.90000
REMARK 3 B22 (A**2) : -15.20000
REMARK 3 B33 (A**2) : 7.30000
REMARK 3 B12 (A**2) : 0.00000
REMARK 3 B13 (A**2) : 0.00000
REMARK 3 B23 (A**2) : 0.00000
REMARK 3
REMARK 3 ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM LUZZATI PLOT (A) : 0.30
REMARK 3 ESD FROM SIGMAA (A) : 0.36
REMARK 3 LOW RESOLUTION CUTOFF (A) : 5.00
REMARK 3
REMARK 3 CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK 3 ESD FROM C-V LUZZATI PLOT (A) : 0.35
REMARK 3 ESD FROM C-V SIGMAA (A) : 0.42
REMARK 3
REMARK 3 RMS DEVIATIONS FROM IDEAL VALUES.
REMARK 3 BOND LENGTHS (A) : 0.008
REMARK 3 BOND ANGLES (DEGREES) : 1.70
REMARK 3 DIHEDRAL ANGLES (DEGREES) : 27.50
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Figure 2 (Table 2 (page 3))

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REMARK 3 IMPROPER ANGLES (DEGREES) : 0.95
REMARK 3
REMARK 3 ISOTROPIC THERMAL MODEL : ANISOTROPIC
REMARK 3
REMARK 3 ISOTROPIC THERMAL FACTOR RESTRAINTS. RMS SIGMA
REMARK 3 MAIN-CHAIN BOND (A**2) : NULL ; NULL
REMARK 3 MAIN-CHAIN ANGLE (A**2) : NULL ; NULL
REMARK 3 SIDE-CHAIN BOND (A**2) : NULL ; NULL
REMARK 3 SIDE-CHAIN ANGLE (A**2) : NULL ; NULL
REMARK 3
REMARK 3 BULK SOLVENT MODELING.
REMARK 3 METHOD USED : NULL
REMARK 3 KSOL : NULL
REMARK 3 BSOL : NULL
REMARK 3
REMARK 3 NCS MODEL : NULL
REMARK 3
REMARK 3 NCS RESTRAINTS. RMS SIGMA/WEIGHT
REMARK 3 GROUP 1 POSITIONAL (A) : NULL ; NULL
REMARK 3 GROUP 1 B-FACTOR (A**2) : NULL ; NULL
REMARK 3
REMARK 3 PARAMETER FILE 1 : NULL
REMARK 3 TOPOLOGY FILE 1 : NULL
REMARK 3
REMARK 3 OTHER REFINEMENT REMARKS: RESIDUES 241-242 WERE NOT LOCATED IN
REMARK 3 THE ELECTRON DENSITY MAP
REMARK 4
REMARK 4 1QZ1 COMPLIES WITH FORMAT V. 2.3, 09-JULY-1998
REMARK 100
REMARK 100 THIS ENTRY HAS BEEN PROCESSED BY RCSB ON 17-SEP-2003.
REMARK 100 THE RCSB ID CODE IS RCSB020242.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200 EXPERIMENT TYPE : X-RAY DIFFRACTION
REMARK 200 DATE OF DATA COLLECTION : 06-NOV-2000; 04-DEC-2000
REMARK 200 TEMPERATURE (KELVIN) : 100.0
REMARK 200 PH : 5.20
REMARK 200 NUMBER OF CRYSTALS USED : 1
REMARK 200
REMARK 200 SYNCHROTRON (Y/N) : Y; N
REMARK 200 RADIATION SOURCE : MAX II ; ROTATING ANODE
REMARK 200 BEAMLINE : I711
REMARK 200 X-RAY GENERATOR MODEL : NULL; HOME SOURCE
REMARK 200 MONOCHROMATIC OR LAUE (M/L) : M
REMARK 200 WAVELENGTH OR RANGE (A) : 1.0526; 1.54
REMARK 200 MONOCHROMATOR : NULL
REMARK 200 OPTICS : NULL
REMARK 200
REMARK 200 DETECTOR TYPE : IMAGE PLATE; IMAGE PLATE
REMARK 200 DETECTOR MANUFACTURER : MARRESEARCH; MARRESEARCH
REMARK 200 INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200 DATA SCALING SOFTWARE : SCALEPACK
REMARK 200
REMARK 200 NUMBER OF UNIQUE REFLECTIONS : 27881
REMARK 200 RESOLUTION RANGE HIGH (A) : 2.000
REMARK 200 RESOLUTION RANGE LOW (A) : 50.000
REMARK 200 REJECTION CRITERIA (SIGMA(I)) : 0.000
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Figure 2 (Table 2 (page 4))

REMARK 200  
REMARK 200 OVERALL.  
REMARK 200 COMPLETENESS FOR RANGE (%) : 99.2  
REMARK 200 DATA REDUNDANCY : 5.900  
REMARK 200 R MERGE (I) : 0.03900  
REMARK 200 R SYM (I) : 0.03900  
REMARK 200 <I/SIGMA(I)> FOR THE DATA SET : 19.6000  
REMARK 200  
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00  
REMARK 200 HIGHEST RESOLUTION SHELL, RANGE LOW (A) : 2.07  
REMARK 200 COMPLETENESS FOR SHELL (%) : 99.4  
REMARK 200 DATA REDUNDANCY IN SHELL : 3.80  
REMARK 200 R MERGE FOR SHELL (I) : 0.20900  
REMARK 200 R SYM FOR SHELL (I) : 0.20900  
REMARK 200 <I/SIGMA(I)> FOR SHELL : 1.400  
REMARK 200  
REMARK 200 DIFFRACTION PROTOCOL: SINGLE WAVELENGTH  
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MOLECULAR REPLACEMENT  
REMARK 200 SOFTWARE USED: AMORE  
REMARK 200 STARTING MODEL: PDB ENTRY 1EPF  
REMARK 200  
REMARK 200 REMARK: NULL  
REMARK 280  
REMARK 280 CRYSTAL  
REMARK 280 SOLVENT CONTENT, VS (%) : NULL  
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS\*\*3/DA) : NULL  
REMARK 280  
REMARK 280 CRYSTALLIZATION CONDITIONS: 14-17% PEG 4000, 450 MM LI SULFATE,  
REMARK 280 100 MM NA ACETATE, PH 5.2, VAPOR DIFFUSION, HANGING DROP,  
REMARK 280 TEMPERATURE 293K  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY  
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: I 21 21 21  
REMARK 290  
REMARK 290 SYMOP SYMMETRY  
REMARK 290 NNNMMM OPERATOR  
REMARK 290 1555 X,Y,Z  
REMARK 290 2555 1/2-X,-Y,1/2+Z  
REMARK 290 3555 -X,1/2+Y,1/2-Z  
REMARK 290 4555 1/2+X,1/2-Y,-Z  
REMARK 290 5555 1/2+X,1/2+Y,1/2+Z  
REMARK 290 6555 -X,1/2-Y,Z  
REMARK 290 7555 1/2-X,Y,-Z  
REMARK 290 8555 X,-Y,1/2-Z  
REMARK 290  
REMARK 290 WHERE NNN -> OPERATOR NUMBER  
REMARK 290 MMM -> TRANSLATION VECTOR  
REMARK 290  
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS  
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM  
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY  
REMARK 290 RELATED MOLECULES.  
REMARK 290 SMTRY1 1 1.000000 0.000000 0.000000 0.000000  
REMARK 290 SMTRY2 1 0.000000 1.000000 0.000000 0.000000  
REMARK 290 SMTRY3 1 0.000000 0.000000 1.000000 0.000000  
REMARK 290 SMTRY1 2 -1.000000 0.000000 0.000000 25.72000

Figure 2 (Table 2 (page 5))

REMARK 290	SMTRY2	2	0.000000	-1.000000	0.000000	0.000000
REMARK 290	SMTRY3	2	0.000000	0.000000	1.000000	74.65000
REMARK 290	SMTRY1	3	-1.000000	0.000000	0.000000	0.00000
REMARK 290	SMTRY2	3	0.000000	1.000000	0.000000	53.88000
REMARK 290	SMTRY3	3	0.000000	0.000000	-1.000000	74.65000
REMARK 290	SMTRY1	4	1.000000	0.000000	0.000000	25.72000
REMARK 290	SMTRY2	4	0.000000	-1.000000	0.000000	53.88000
REMARK 290	SMTRY3	4	0.000000	0.000000	-1.000000	0.00000
REMARK 290	SMTRY1	5	1.000000	0.000000	0.000000	25.72000
REMARK 290	SMTRY2	5	0.000000	1.000000	0.000000	53.88000
REMARK 290	SMTRY3	5	0.000000	0.000000	1.000000	74.65000
REMARK 290	SMTRY1	6	-1.000000	0.000000	0.000000	0.00000
REMARK 290	SMTRY2	6	0.000000	-1.000000	0.000000	53.88000
REMARK 290	SMTRY3	6	0.000000	0.000000	1.000000	0.00000
REMARK 290	SMTRY1	7	-1.000000	0.000000	0.000000	25.72000
REMARK 290	SMTRY2	7	0.000000	1.000000	0.000000	0.00000
REMARK 290	SMTRY3	7	0.000000	0.000000	-1.000000	0.00000
REMARK 290	SMTRY1	8	1.000000	0.000000	0.000000	0.00000
REMARK 290	SMTRY2	8	0.000000	-1.000000	0.000000	0.00000
REMARK 290	SMTRY3	8	0.000000	0.000000	-1.000000	74.65000
REMARK 290						
REMARK 290	REMARK: NULL					
REMARK 300						
REMARK 300	BIOMOLECULE: 1					
REMARK 300	THIS ENTRY CONTAINS THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT					
REMARK 300	WHICH CONSISTS OF 1 CHAIN(S). SEE REMARK 350 FOR					
REMARK 300	INFORMATION ON GENERATING THE BIOLOGICAL MOLECULE(S).					
REMARK 350						
REMARK 350	GENERATING THE BIOMOLECULE					
REMARK 350	COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN					
REMARK 350	BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE					
REMARK 350	MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS					
REMARK 350	GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND					
REMARK 350	CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.					
REMARK 350						
REMARK 350	BIOMOLECULE: 1					
REMARK 350	APPLY THE FOLLOWING TO CHAINS: A					
REMARK 350	BIOMT1	1	1.000000	0.000000	0.000000	0.00000
REMARK 350	BIOMT2	1	0.000000	1.000000	0.000000	0.00000
REMARK 350	BIOMT3	1	0.000000	0.000000	1.000000	0.00000
REMARK 465						
REMARK 465	MISSING RESIDUES					
REMARK 465	THE FOLLOWING RESIDUES WERE NOT LOCATED IN THE					
REMARK 465	EXPERIMENT. (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN					
REMARK 465	IDENTIFIER; SSSEQ=SEQUENCE NUMBER; I=INSERTION CODE.)					
REMARK 465						
REMARK 465	M	RES	C	SSSEQI		
REMARK 465		ARG	A	-2		
REMARK 465		GLU	A	239		
REMARK 465		GLU	A	240		
REMARK 500						
REMARK 500	GEOMETRY AND STEREOCHEMISTRY					
REMARK 500	SUBTOPIC: COVALENT BOND ANGLES					
REMARK 500						
REMARK 500	THE STEREOCHEMICAL PARAMETERS OF THE FOLLOWING RESIDUES					
REMARK 500	HAVE VALUES WHICH DEVIATE FROM EXPECTED VALUES BY MORE					
REMARK 500	THAN 6* $\sigma$ (M=MODEL NUMBER; RES=RESIDUE NAME; C=CHAIN					

Figure 2 (Table 2 (page 6))

REMARK 500 IDENTIFIER; SSEQ=SEQUENCE NUMBER; I=INSERTION CODE).

REMARK 500

REMARK 500 STANDARD TABLE:

REMARK 500 FORMAT: (10X,I3,1X,A3,1X,A1,I4,A1,3(1X,A4,2X),12X,F5.1)

REMARK 500

REMARK 500 EXPECTED VALUES: ENGH AND HUBER, 1991

REMARK 500

REMARK 500	M	RES	CSSEQI	ATM1	ATM2	ATM3	
REMARK 500	LEU	A	1	N	-	CA	- C ANGL. DEV. = 11.0 DEGREES
REMARK 500	ASP	A	27	N	-	CA	- C ANGL. DEV. = 11.4 DEGREES
REMARK 500	ALA	A	28	N	-	CA	- C ANGL. DEV. = -17.5 DEGREES
REMARK 500	LYS	A	29	N	-	CA	- C ANGL. DEV. = 12.7 DEGREES
REMARK 500	ASP	A	56	N	-	CA	- C ANGL. DEV. = -11.4 DEGREES
REMARK 500	ALA	A	89	N	-	CA	- C ANGL. DEV. = -10.5 DEGREES
REMARK 500	GLN	A	108	N	-	CA	- C ANGL. DEV. = -10.5 DEGREES
REMARK 500	THR	A	129	N	-	CA	- C ANGL. DEV. = -11.4 DEGREES
REMARK 500	ASP	A	138	N	-	CA	- C ANGL. DEV. = -11.4 DEGREES
REMARK 500	ASP	A	144	N	-	CA	- C ANGL. DEV. = -20.1 DEGREES
REMARK 500	THR	A	194	N	-	CA	- C ANGL. DEV. = -11.0 DEGREES
REMARK 500	ARG	A	257	N	-	CA	- C ANGL. DEV. = 17.3 DEGREES

REMARK 525

REMARK 525 SOLVENT

REMARK 525 THE FOLLOWING SOLVENT MOLECULES LIE FARTHER THAN EXPECTED

REMARK 525 FROM THE PROTEIN OR NUCLEIC ACID MOLECULE AND MAY BE

REMARK 525 ASSOCIATED WITH A SYMMETRY RELATED MOLECULE (M=MODEL

REMARK 525 NUMBER; RES=RESIDUE NAME; C=CHAIN IDENTIFIER; SSEQ=SEQUENCE

REMARK 525 NUMBER; I=INSERTION CODE):

REMARK 525

REMARK 525	M	RES	CSSEQI	
REMARK 525	HOH		64	DISTANCE = 5.56 ANGSTROMS
REMARK 525	HOH		66	DISTANCE = 7.20 ANGSTROMS
REMARK 525	HOH		75	DISTANCE = 10.03 ANGSTROMS

REMARK 900

REMARK 900 RELATED ENTRIES

REMARK 900 RELATED ID: 2NCM RELATED DB: PDB

REMARK 900 NMR STRUCTURE OF THE FIRST IMMUNOGLOBULIN DOMAIN OF THE

REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)

REMARK 900 RELATED ID: 3NCM RELATED DB: PDB

REMARK 900 NMR STRUCTURE OF THE SECOND IMMUNOGLOBULIN DOMAIN OF THE

REMARK 900 NEURAL CELL ADHESION MOLECULE (NCAM)

REMARK 900 RELATED ID: 1EPF RELATED DB: PDB

REMARK 900 CRYSTAL STRUCTURE OF THE TWO N-TERMINAL IMMUNOGLOBULIN

REMARK 900 DOMAINS OF THE NEURAL CELL ADHESION MOLECULE (NCAM)

REMARK 999

REMARK 999 SEQUENCE

REMARK 999 RESIDUES -2, 239 AND 240 WERE NOT VISIBLE IN

REMARK 999 THE ELECTRON DENSITY.

DBREF	1QZ1	A	1	289	SWS	P13596	NCA1_RAT	20	308
SEQADV	1QZ1	ARG	A	-2	SWS	P13596		CLONING	ARTIFACT
SEQADV	1QZ1	VAL	A	-1	SWS	P13596		CLONING	ARTIFACT
SEQRES	1	A	291	ARG	VAL	LEU	GLN	VAL	ASP
SEQRES	2	A	291	ILE	SER	VAL	GLY	GLU	SER
SEQRES	3	A	291	ALA	GLY	ASP	ALA	LYS	ASP
SEQRES	4	A	291	PRO	ASN	GLY	GLU	LYS	LEU
SEQRES	5	A	291	SER	VAL	VAL	TRP	ASN	ASP
SEQRES	6	A	291	ILE	TYR	ASN	ALA	ASN	ILE
SEQRES	7	A	291	CYS	VAL	VAL	THR	ALA	GLU

Figure 2 (Table 2 (page 7))

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SEQRES  8  A 291  THR VAL ASN VAL LYS ILE PHE GLN LYS LEU MET PHE LYS
SEQRES  9  A 291  ASN ALA PRO THR PRO GLN GLU PHE LYS GLU GLY GLU ASP
SEQRES 10  A 291  ALA VAL ILE VAL CYS ASP VAL VAL SER SER LEU PRO PRO
SEQRES 11  A 291  THR ILE ILE TRP LYS HIS LYS GLY ARG ASP VAL ILE LEU
SEQRES 12  A 291  LYS LYS ASP VAL ARG PHE ILE VAL LEU SER ASN ASN TYR
SEQRES 13  A 291  LEU GLN ILE ARG GLY ILE LYS LYS THR ASP GLU GLY THR
SEQRES 14  A 291  TYR ARG CYS GLU GLY ARG ILE LEU ALA ARG GLY GLU ILE
SEQRES 15  A 291  ASN PHE LYS ASP ILE GLN VAL ILE VAL ASN VAL PRO PRO
SEQRES 16  A 291  THR VAL GLN ALA ARG GLN SER ILE VAL ASN ALA THR ALA
SEQRES 17  A 291  ASN LEU GLY GLN SER VAL THR LEU VAL CYS ASP ALA ASP
SEQRES 18  A 291  GLY PHE PRO GLU PRO THR MET SER TRP THR LYS ASP GLY
SEQRES 19  A 291  GLU PRO ILE GLU ASN GLU GLU GLU ASP ASP GLU LYS HIS
SEQRES 20  A 291  ILE PHE SER ASP ASP SER SER GLU LEU THR ILE ARG ASN
SEQRES 21  A 291  VAL ASP LYS ASN ASP GLU ALA GLU TYR VAL CYS ILE ALA
SEQRES 22  A 291  GLU ASN LYS ALA GLY GLU GLN ASP ALA SER ILE HIS LEU
SEQRES 23  A 291  LYS VAL PHE ALA LYS
FORMUL  2  HOH      *265(H2 O1)
HELIX   1  1 ASN A   68 ALA A   72 5
HELIX   2  2 LYS A  161 GLU A  165 5
HELIX   3  3 ASP A  260 GLU A  264 5
SHEET   1  A 4 VAL A   3 VAL A   6 0
SHEET   2  A 4 LYS A  18 VAL A  24 -1 O GLN A  23 N ASP A  4
SHEET   3  A 4 SER A  59 ILE A  64 -1 O ILE A  64 N LYS A 18
SHEET   4  A 4 ILE A  50 ASP A  56 -1 N VAL A  53 O THR A 61
SHEET   1  B 4 GLY A  10 SER A  13 0
SHEET   2  B 4 GLN A  86 PHE A  96 1 O LYS A  94 N GLY A  0
SHEET   3  B 4 GLY A  73 THR A  80 -1 N VAL A  79 O SER A 87
SHEET   4  B 4 ASP A  32 PHE A  36 -1 N SER A  34 O VAL A 78
SHEET   1  C 2 MET A 100 ASN A 103 0
SHEET   2  C 2 ASP A 121 VAL A 123 -1 O ASP A 121 N ASN A 103
SHEET   1  D 4 GLN A 108 LYS A 111 0
SHEET   2  D 4 GLU A 179 ALA A 197 1 O ASN A 190 N PHE A 110
SHEET   3  D 4 GLY A 166 ILE A 174 -1 N GLY A 166 O VAL A 187
SHEET   4  D 4 THR A 129 HIS A 134 -1 N LYS A 133 O ARG A 169
SHEET   1  E 5 GLN A 108 LYS A 111 0
SHEET   2  E 5 GLU A 179 ALA A 197 1 O ASN A 190 N PHE A 110
SHEET   3  E 5 VAL A 212 PHE A 221 -1 O ASP A 217 N GLN A 196
SHEET   4  E 5 GLU A 253 ILE A 256 -1 O LEU A 254 N LEU A 214
SHEET   5  E 5 HIS A 245 PHE A 247 -1 N ILE A 246 O THR A 255
SHEET   1  F 3 ALA A 116 ILE A 118 0
SHEET   2  F 3 LEU A 155 ILE A 157 -1 O ILE A 157 N ALA A 116
SHEET   3  F 3 PHE A 147 VAL A 149 -1 N ILE A 148 O GLN A 156
SHEET   1  G 5 ILE A 201 THR A 205 0
SHEET   2  G 5 GLY A 276 PHE A 287 1 O PHE A 287 N ALA A 204
SHEET   3  G 5 ALA A 265 ASN A 273 -1 N TYR A 267 O ILE A 282
SHEET   4  G 5 THR A 225 LYS A 230 -1 N SER A 227 O ILE A 270
SHEET   5  G 5 GLU A 233 PRO A 234 -1 O GLU A 233 N LYS A 230
SSBOND  1  CYS A   22 CYS A   77
SSBOND  2  CYS A  120 CYS A  170
SSBOND  3  CYS A  216 CYS A  269
CISPEP  1  VAL A   6 PRO A   7 0 -0.41
CISPEP  2  THR A 106 PRO A 107 0 -0.64
CISPEP  3  PHE A 221 PRO A 222 0 -0.72
CRYST1  51.440 107.760 149.300 90.00 90.00 90.00 I 21 21 21 8
ORIGX1  1.000000 0.000000 0.000000 0.000000
ORIGX2  0.000000 1.000000 0.000000 0.000000
ORIGX3  0.000000 0.000000 1.000000 0.000000

```



Figure 2 (Table 2 (page 8))

SCALE1				0.019440	0.000000	0.000000	0.000000	
SCALE2				0.000000	0.009280	0.000000	0.000000	
SCALE3				0.000000	0.000000	0.006698	0.000000	
ATOM	1	N	VAL	A	-1	21.197	71.826	-24.060 1.00110.27 N
ATOM	2	CA	VAL	A	-1	21.299	70.596	-24.891 1.00112.18 C
ATOM	3	C	VAL	A	-1	20.583	69.411	-24.264 1.00111.88 C
ATOM	4	O	VAL	A	-1	19.491	69.531	-23.699 1.00113.09 O
ATOM	5	CB	VAL	A	-1	22.778	70.161	-25.114 1.00111.00 C
ATOM	6	CG1	VAL	A	-1	23.591	71.324	-25.633 1.00109.72 C
ATOM	7	CG2	VAL	A	-1	23.374	69.625	-23.817 1.00106.12 C
ATOM	8	N	LEU	A	1	21.255	68.270	-24.364 1.00107.51 N
ATOM	9	CA	LEU	A	1	20.778	66.981	-23.905 1.00100.28 C
ATOM	10	C	LEU	A	1	20.360	66.739	-22.465 1.00 94.24 C
ATOM	11	O	LEU	A	1	20.985	67.227	-21.518 1.00 93.77 O
ATOM	12	CB	LEU	A	1	21.808	65.936	-24.296 1.00100.43 C
ATOM	13	CG	LEU	A	1	21.297	64.909	-25.303 1.00103.11 C
ATOM	14	CD1	LEU	A	1	20.253	65.528	-26.233 1.00106.65 C
ATOM	15	CD2	LEU	A	1	22.475	64.366	-26.088 1.00101.88 C
ATOM	16	N	GLN	A	2	19.299	65.946	-22.328 1.00 87.47 N
ATOM	17	CA	GLN	A	2	18.771	65.575	-21.028 1.00 86.76 C
ATOM	18	C	GLN	A	2	18.937	64.075	-20.822 1.00 80.18 C
ATOM	19	O	GLN	A	2	18.520	63.264	-21.656 1.00 82.58 O
ATOM	20	CB	GLN	A	2	17.292	65.950	-20.902 1.00 89.86 C
ATOM	21	CG	GLN	A	2	16.819	65.996	-19.458 1.00102.22 C
ATOM	22	CD	GLN	A	2	17.932	66.444	-18.500 1.00109.49 C
ATOM	23	OE1	GLN	A	2	18.786	67.260	-18.859 1.00112.97 O
ATOM	24	NE2	GLN	A	2	17.917	65.917	-17.275 1.00110.51 N
ATOM	25	N	VAL	A	3	19.572	63.716	-19.714 1.00 68.44 N
ATOM	26	CA	VAL	A	3	19.790	62.317	-19.375 1.00 65.80 C
ATOM	27	C	VAL	A	3	19.290	62.058	-17.959 1.00 63.80 C
ATOM	28	O	VAL	A	3	19.588	62.816	-17.029 1.00 61.99 O
ATOM	29	CB	VAL	A	3	21.291	61.919	-19.495 1.00 70.09 C
ATOM	30	CG1	VAL	A	3	22.157	62.831	-18.653 1.00 66.37 C
ATOM	31	CG2	VAL	A	3	21.477	60.475	-19.072 1.00 53.43 C
ATOM	32	N	ASP	A	4	18.511	60.992	-17.807 1.00 59.47 N
ATOM	33	CA	ASP	A	4	17.957	60.635	-16.507 1.00 62.16 C
ATOM	34	C	ASP	A	4	18.056	59.137	-16.281 1.00 61.45 C
ATOM	35	O	ASP	A	4	17.973	58.337	-17.222 1.00 54.28 O
ATOM	36	CB	ASP	A	4	16.490	61.064	-16.410 1.00 57.25 C
ATOM	37	CG	ASP	A	4	16.312	62.564	-16.536 1.00 81.12 C
ATOM	38	OD1	ASP	A	4	16.784	63.302	-15.644 1.00 87.44 O
ATOM	39	OD2	ASP	A	4	15.702	63.010	-17.531 1.00 84.62 O
ATOM	40	N	ILE	A	5	18.226	58.760	-15.024 1.00 54.90 N
ATOM	41	CA	ILE	A	5	18.324	57.360	-14.692 1.00 47.24 C
ATOM	42	C	ILE	A	5	17.134	56.965	-13.832 1.00 49.02 C
ATOM	43	O	ILE	A	5	16.846	57.619	-12.826 1.00 47.37 O
ATOM	44	CB	ILE	A	5	19.625	57.077	-13.934 1.00 42.30 C
ATOM	45	CG1	ILE	A	5	20.823	57.333	-14.849 1.00 48.79 C
ATOM	46	CG2	ILE	A	5	19.638	55.615	-13.450 1.00 40.90 C
ATOM	47	CD1	ILE	A	5	22.158	57.356	-14.118 1.00 47.66 C
ATOM	48	N	VAL	A	6	16.445	55.900	-14.233 1.00 48.39 N
ATOM	49	CA	VAL	A	6	15.300	55.401	-13.480 1.00 48.78 C
ATOM	50	C	VAL	A	6	15.545	53.939	-13.119 1.00 52.24 C
ATOM	51	O	VAL	A	6	15.905	53.130	-13.980 1.00 51.37 O
ATOM	52	CB	VAL	A	6	14.008	55.484	-14.299 1.00 55.65 C
ATOM	53	CG1	VAL	A	6	12.857	54.882	-13.515 1.00 53.36 C
ATOM	54	CG2	VAL	A	6	13.712	56.928	-14.637 1.00 64.21 C

Figure 2 (Table 2 (page 9))

ATOM	55	N	PRO	A	7	15.418	53.594	-11.830	1.00	44.55	N
ATOM	56	CA	PRO	A	7	15.074	54.460	-10.692	1.00	44.98	C
ATOM	57	C	PRO	A	7	16.225	55.428	-10.411	1.00	52.07	C
ATOM	58	O	PRO	A	7	17.391	55.112	-10.662	1.00	47.92	O
ATOM	59	CB	PRO	A	7	14.842	53.462	-9.556	1.00	50.48	C
ATOM	60	CG	PRO	A	7	15.718	52.291	-9.944	1.00	45.69	C
ATOM	61	CD	PRO	A	7	15.446	52.181	-11.420	1.00	40.86	C
ATOM	62	N	SER	A	8	15.894	56.604	-9.893	1.00	46.31	N
ATOM	63	CA	SER	A	8	16.889	57.635	-9.634	1.00	49.55	C
ATOM	64	C	SER	A	8	17.921	57.250	-8.592	1.00	53.48	C
ATOM	65	O	SER	A	8	18.995	57.857	-8.515	1.00	54.87	O
ATOM	66	CB	SER	A	8	16.198	58.940	-9.236	1.00	55.09	C
ATOM	67	OG	SER	A	8	15.363	58.753	-8.111	1.00	61.93	O
ATOM	68	N	GLN	A	9	17.597	56.255	-7.776	1.00	46.60	N
ATOM	69	CA	GLN	A	9	18.538	55.781	-6.771	1.00	47.40	C
ATOM	70	C	GLN	A	9	18.204	54.335	-6.448	1.00	44.46	C
ATOM	71	O	GLN	A	9	17.103	53.864	-6.739	1.00	52.34	O
ATOM	72	CB	GLN	A	9	18.494	56.658	-5.515	1.00	58.55	C
ATOM	73	CG	GLN	A	9	17.103	56.860	-4.900	1.00	65.92	C
ATOM	74	CD	GLN	A	9	17.149	57.765	-3.665	1.00	81.94	C
ATOM	75	OE1	GLN	A	9	17.878	57.484	-2.713	1.00	86.13	O
ATOM	76	NE2	GLN	A	9	16.374	58.853	-3.678	1.00	82.96	N
ATOM	77	N	GLY	A	10	19.157	53.606	-5.883	1.00	46.46	N
ATOM	78	CA	GLY	A	10	18.868	52.215	-5.589	1.00	50.99	C
ATOM	79	C	GLY	A	10	19.637	51.600	-4.442	1.00	48.97	C
ATOM	80	O	GLY	A	10	20.719	52.048	-4.070	1.00	46.47	O
ATOM	81	N	GLU	A	11	19.051	50.559	-3.871	1.00	54.04	N
ATOM	82	CA	GLU	A	11	19.684	49.842	-2.778	1.00	54.83	C
ATOM	83	C	GLU	A	11	19.560	48.362	-3.127	1.00	47.65	C
ATOM	84	O	GLU	A	11	18.499	47.918	-3.557	1.00	47.49	O
ATOM	85	CB	GLU	A	11	18.970	50.150	-1.456	1.00	49.30	C
ATOM	86	CG	GLU	A	11	19.627	49.508	-0.255	1.00	67.71	C
ATOM	87	CD	GLU	A	11	19.026	49.974	1.061	1.00	68.83	C
ATOM	88	OE1	GLU	A	11	17.829	49.704	1.305	1.00	70.78	O
ATOM	89	OE2	GLU	A	11	19.758	50.620	1.843	1.00	73.96	O
ATOM	90	N	ILE	A	12	20.636	47.599	-2.965	1.00	44.79	N
ATOM	91	CA	ILE	A	12	20.587	46.178	-3.302	1.00	43.25	C
ATOM	92	C	ILE	A	12	21.164	45.332	-2.185	1.00	49.76	C
ATOM	93	O	ILE	A	12	22.261	45.610	-1.692	1.00	45.49	O
ATOM	94	CB	ILE	A	12	21.402	45.856	-4.562	1.00	46.25	C
ATOM	95	CG1	ILE	A	12	21.182	46.938	-5.621	1.00	48.07	C
ATOM	96	CG2	ILE	A	12	20.984	44.481	-5.114	1.00	40.48	C
ATOM	97	CD1	ILE	A	12	22.125	46.814	-6.795	1.00	44.46	C
ATOM	98	N	SER	A	13	20.421	44.296	-1.796	1.00	50.25	N
ATOM	99	CA	SER	A	13	20.880	43.384	-0.755	1.00	49.85	C
ATOM	100	C	SER	A	13	21.869	42.416	-1.385	1.00	41.84	C
ATOM	101	O	SER	A	13	21.690	41.973	-2.526	1.00	43.99	O
ATOM	102	CB	SER	A	13	19.707	42.608	-0.156	1.00	48.85	C
ATOM	103	OG	SER	A	13	20.157	41.794	0.916	1.00	55.47	O
ATOM	104	N	VAL	A	14	22.926	42.114	-0.644	1.00	50.09	N
ATOM	105	CA	VAL	A	14	23.955	41.214	-1.126	1.00	48.58	C
ATOM	106	C	VAL	A	14	23.358	39.962	-1.742	1.00	53.11	C
ATOM	107	O	VAL	A	14	22.481	39.320	-1.165	1.00	54.25	O
ATOM	108	CB	VAL	A	14	24.924	40.814	0.004	1.00	51.58	C
ATOM	109	CG1	VAL	A	14	25.880	39.739	-0.479	1.00	51.54	C
ATOM	110	CG2	VAL	A	14	25.702	42.027	0.455	1.00	51.93	C
ATOM	111	N	GLY	A	15	23.841	39.636	-2.935	1.00	45.67	N

Figure 2 (Table 2 (page 10))

ATOM	112	CA	GLY	A	15	23.367	38.471	-3.643	1.00	45.80	C
ATOM	113	C	GLY	A	15	22.174	38.738	-4.546	1.00	49.51	C
ATOM	114	O	GLY	A	15	21.845	37.910	-5.395	1.00	44.42	O
ATOM	115	N	GLU	A	16	21.516	39.885	-4.390	1.00	48.69	N
ATOM	116	CA	GLU	A	16	20.360	40.167	-5.239	1.00	44.66	C
ATOM	117	C	GLU	A	16	20.712	41.010	-6.459	1.00	38.83	C
ATOM	118	O	GLU	A	16	21.874	41.355	-6.672	1.00	41.87	O
ATOM	119	CB	GLU	A	16	19.239	40.800	-4.403	1.00	44.40	C
ATOM	120	CG	GLU	A	16	18.799	39.848	-3.289	1.00	57.20	C
ATOM	121	CD	GLU	A	16	17.666	40.373	-2.428	1.00	67.70	C
ATOM	122	OE1	GLU	A	16	17.111	41.448	-2.739	1.00	72.10	O
ATOM	123	OE2	GLU	A	16	17.328	39.695	-1.433	1.00	77.10	O
ATOM	124	N	SER	A	17	19.712	41.319	-7.274	1.00	38.10	N
ATOM	125	CA	SER	A	17	19.950	42.068	-8.496	1.00	39.72	C
ATOM	126	C	SER	A	17	19.039	43.283	-8.655	1.00	43.71	C
ATOM	127	O	SER	A	17	17.960	43.330	-8.074	1.00	48.43	O
ATOM	128	CB	SER	A	17	19.787	41.125	-9.694	1.00	42.04	C
ATOM	129	OG	SER	A	17	20.672	40.016	-9.592	1.00	49.33	O
ATOM	130	N	LYS	A	18	19.491	44.273	-9.427	1.00	39.31	N
ATOM	131	CA	LYS	A	18	18.725	45.495	-9.689	1.00	40.44	C
ATOM	132	C	LYS	A	18	19.194	46.068	-11.004	1.00	36.17	C
ATOM	133	O	LYS	A	18	20.310	45.799	-11.447	1.00	41.18	O
ATOM	134	CB	LYS	A	18	18.944	46.552	-8.603	1.00	45.93	C
ATOM	135	CG	LYS	A	18	17.902	46.558	-7.506	1.00	63.96	C
ATOM	136	CD	LYS	A	18	17.343	47.954	-7.318	1.00	77.99	C
ATOM	137	CE	LYS	A	18	16.408	48.029	-6.120	1.00	91.67	C
ATOM	138	NZ	LYS	A	18	15.285	47.049	-6.198	1.00	104.95	N
ATOM	139	N	PHE	A	19	18.355	46.866	-11.632	1.00	39.73	N
ATOM	140	CA	PHE	A	19	18.758	47.445	-12.889	1.00	42.56	C
ATOM	141	C	PHE	A	19	18.382	48.903	-12.907	1.00	45.52	C
ATOM	142	O	PHE	A	19	17.535	49.352	-12.123	1.00	41.88	O
ATOM	143	CB	PHE	A	19	18.131	46.681	-14.058	1.00	37.12	C
ATOM	144	CG	PHE	A	19	16.658	46.890	-14.220	1.00	41.51	C
ATOM	145	CD1	PHE	A	19	16.175	47.864	-15.090	1.00	45.13	C
ATOM	146	CD2	PHE	A	19	15.742	46.075	-13.547	1.00	42.50	C
ATOM	147	CE1	PHE	A	19	14.794	48.006	-15.310	1.00	44.84	C
ATOM	148	CE2	PHE	A	19	14.377	46.212	-13.759	1.00	43.30	C
ATOM	149	CZ	PHE	A	19	13.899	47.182	-14.639	1.00	41.52	C
ATOM	150	N	PHE	A	20	19.020	49.637	-13.813	1.00	37.54	N
ATOM	151	CA	PHE	A	20	18.816	51.062	-13.938	1.00	38.86	C
ATOM	152	C	PHE	A	20	18.816	51.437	-15.408	1.00	46.44	C
ATOM	153	O	PHE	A	20	19.702	51.035	-16.165	1.00	47.88	O
ATOM	154	CB	PHE	A	20	19.948	51.798	-13.205	1.00	36.96	C
ATOM	155	CG	PHE	A	20	20.112	51.368	-11.784	1.00	46.76	C
ATOM	156	CD1	PHE	A	20	20.904	50.267	-11.460	1.00	48.63	C
ATOM	157	CD2	PHE	A	20	19.427	52.027	-10.765	1.00	42.55	C
ATOM	158	CE1	PHE	A	20	21.008	49.826	-10.138	1.00	46.86	C
ATOM	159	CE2	PHE	A	20	19.525	51.591	-9.436	1.00	40.53	C
ATOM	160	CZ	PHE	A	20	20.317	50.489	-9.126	1.00	44.32	C
ATOM	161	N	LEU	A	21	17.816	52.209	-15.806	1.00	46.01	N
ATOM	162	CA	LEU	A	21	17.680	52.649	-17.189	1.00	49.63	C
ATOM	163	C	LEU	A	21	18.131	54.087	-17.360	1.00	46.97	C
ATOM	164	O	LEU	A	21	17.602	54.990	-16.719	1.00	43.22	O
ATOM	165	CB	LEU	A	21	16.218	52.530	-17.641	1.00	54.55	C
ATOM	166	CG	LEU	A	21	15.857	53.049	-19.040	1.00	57.21	C
ATOM	167	CD1	LEU	A	21	16.625	52.281	-20.096	1.00	58.14	C
ATOM	168	CD2	LEU	A	21	14.365	52.891	-19.274	1.00	55.27	C

Figure 2 (Table 2 (page 11))

ATOM	169	N	CYS	A	22	19.122	54.291	-18.218	1.00	46.45	N
ATOM	170	CA	CYS	A	22	19.615	55.628	-18.506	1.00	48.52	C
ATOM	171	C	CYS	A	22	18.920	56.056	-19.788	1.00	54.42	C
ATOM	172	O	CYS	A	22	19.157	55.478	-20.848	1.00	51.82	O
ATOM	173	CB	CYS	A	22	21.115	55.601	-18.730	1.00	49.72	C
ATOM	174	SG	CYS	A	22	21.827	57.215	-19.167	1.00	55.16	S
ATOM	175	N	GLN	A	23	18.069	57.071	-19.689	1.00	59.11	N
ATOM	176	CA	GLN	A	23	17.312	57.546	-20.837	1.00	66.68	C
ATOM	177	C	GLN	A	23	17.718	58.941	-21.314	1.00	63.21	C
ATOM	178	O	GLN	A	23	17.951	59.839	-20.509	1.00	57.50	O
ATOM	179	CB	GLN	A	23	15.825	57.547	-20.482	1.00	69.27	C
ATOM	180	CG	GLN	A	23	14.900	57.940	-21.618	1.00	83.38	C
ATOM	181	CD	GLN	A	23	14.575	56.779	-22.549	1.00	90.68	C
ATOM	182	OE1	GLN	A	23	14.251	55.685	-22.089	1.00	97.59	O
ATOM	183	NE2	GLN	A	23	14.642	57.016	-23.861	1.00	95.34	N
ATOM	184	N	VAL	A	24	17.799	59.118	-22.629	1.00	67.26	N
ATOM	185	CA	VAL	A	24	18.145	60.415	-23.197	1.00	74.82	C
ATOM	186	C	VAL	A	24	16.857	61.028	-23.739	1.00	75.90	C
ATOM	187	O	VAL	A	24	16.039	60.338	-24.356	1.00	76.41	O
ATOM	188	CB	VAL	A	24	19.178	60.285	-24.343	1.00	77.43	C
ATOM	189	CG1	VAL	A	24	19.560	61.657	-24.852	1.00	77.38	C
ATOM	190	CG2	VAL	A	24	20.418	59.547	-23.856	1.00	81.07	C
ATOM	191	N	ALA	A	25	16.685	62.324	-23.500	1.00	82.73	N
ATOM	192	CA	ALA	A	25	15.490	63.053	-23.933	1.00	92.22	C
ATOM	193	C	ALA	A	25	15.455	63.428	-25.424	1.00	99.21	C
ATOM	194	O	ALA	A	25	16.491	63.734	-26.019	1.00	99.63	O
ATOM	195	CB	ALA	A	25	15.326	64.307	-23.078	1.00	89.44	C
ATOM	196	N	GLY	A	26	14.249	63.405	-26.002	1.00	107.66	N
ATOM	197	CA	GLY	A	26	14.040	63.735	-27.410	1.00	117.13	C
ATOM	198	C	GLY	A	26	14.697	62.739	-28.348	1.00	123.74	C
ATOM	199	O	GLY	A	26	14.060	62.088	-29.188	1.00	126.85	O
ATOM	200	N	ASP	A	27	16.010	62.671	-28.187	1.00	127.93	N
ATOM	201	CA	ASP	A	27	16.915	61.795	-28.897	1.00	131.73	C
ATOM	202	C	ASP	A	27	17.049	61.809	-30.410	1.00	132.38	C
ATOM	203	O	ASP	A	27	16.518	60.944	-31.112	1.00	134.43	O
ATOM	204	CB	ASP	A	27	16.721	60.353	-28.433	1.00	133.67	C
ATOM	205	CG	ASP	A	27	17.976	59.540	-28.620	1.00	136.05	C
ATOM	206	OD1	ASP	A	27	19.011	60.177	-28.888	1.00	137.46	O
ATOM	207	OD2	ASP	A	27	17.940	58.305	-28.501	1.00	138.22	O
ATOM	208	N	ALA	A	28	17.776	62.812	-30.894	1.00	130.01	N
ATOM	209	CA	ALA	A	28	18.098	62.888	-32.301	1.00	127.19	C
ATOM	210	C	ALA	A	28	19.203	61.826	-32.208	1.00	125.97	C
ATOM	211	O	ALA	A	28	19.562	61.453	-31.091	1.00	125.76	O
ATOM	212	CB	ALA	A	28	18.672	64.248	-32.657	1.00	123.21	C
ATOM	213	N	LYS	A	29	19.777	61.332	-33.300	1.00	124.23	N
ATOM	214	CA	LYS	A	29	20.754	60.267	-33.095	1.00	120.04	C
ATOM	215	C	LYS	A	29	22.237	60.419	-33.356	1.00	114.93	C
ATOM	216	O	LYS	A	29	22.773	61.503	-33.593	1.00	109.02	O
ATOM	217	CB	LYS	A	29	20.254	58.988	-33.777	1.00	124.97	C
ATOM	218	CG	LYS	A	29	19.095	58.340	-33.030	1.00	125.66	C
ATOM	219	CD	LYS	A	29	18.639	57.047	-33.674	1.00	125.32	C
ATOM	220	CE	LYS	A	29	17.462	56.460	-32.915	1.00	120.15	C
ATOM	221	NZ	LYS	A	29	16.388	57.477	-32.740	1.00	120.03	N
ATOM	222	N	ASP	A	30	22.875	59.260	-33.286	1.00	110.94	N
ATOM	223	CA	ASP	A	30	24.297	59.108	-33.440	1.00	108.72	C
ATOM	224	C	ASP	A	30	25.004	59.738	-32.257	1.00	102.56	C
ATOM	225	O	ASP	A	30	25.869	60.592	-32.425	1.00	101.55	O

Figure 2 (Table 2 (page 12))

ATOM	226	CB	ASP	A	30	24.800	59.729	-34.740	1.00114.65	C
ATOM	227	CG	ASP	A	30	25.573	58.735	-35.584	1.00121.84	C
ATOM	228	OD1	ASP	A	30	26.219	57.833	-35.001	1.00126.50	O
ATOM	229	OD2	ASP	A	30	25.543	58.853	-36.824	1.00125.16	O
ATOM	230	N	LYS	A	31	24.602	59.339	-31.055	1.00	90.62 N
ATOM	231	CA	LYS	A	31	25.252	59.820	-29.845	1.00	86.82 C
ATOM	232	C	LYS	A	31	25.645	58.547	-29.120	1.00	76.37 C
ATOM	233	O	LYS	A	31	25.000	57.512	-29.280	1.00	76.59 O
ATOM	234	CB	LYS	A	31	24.315	60.658	-28.965	1.00	87.55 C
ATOM	235	CG	LYS	A	31	23.238	59.873	-28.261	1.00	90.62 C
ATOM	236	CD	LYS	A	31	21.906	60.210	-28.856	1.00	90.82 C
ATOM	237	CE	LYS	A	31	21.081	58.968	-28.999	1.00	94.15 C
ATOM	238	NZ	LYS	A	31	20.424	58.901	-30.339	1.00	96.17 N
ATOM	239	N	ASP	A	32	26.711	58.620	-28.341	1.00	66.33 N
ATOM	240	CA	ASP	A	32	27.202	57.467	-27.607	1.00	64.69 C
ATOM	241	C	ASP	A	32	26.732	57.503	-26.163	1.00	57.45 C
ATOM	242	O	ASP	A	32	26.707	58.563	-25.532	1.00	61.27 O
ATOM	243	CB	ASP	A	32	28.740	57.448	-27.669	1.00	59.49 C
ATOM	244	CG	ASP	A	32	29.372	56.362	-26.791	1.00	67.93 C
ATOM	245	OD1	ASP	A	32	29.627	56.626	-25.589	1.00	51.53 O
ATOM	246	OD2	ASP	A	32	29.626	55.248	-27.308	1.00	61.79 O
ATOM	247	N	ILE	A	33	26.336	56.342	-25.657	1.00	54.91 N
ATOM	248	CA	ILE	A	33	25.911	56.210	-24.271	1.00	52.46 C
ATOM	249	C	ILE	A	33	26.823	55.173	-23.640	1.00	53.58 C
ATOM	250	O	ILE	A	33	26.875	54.022	-24.083	1.00	50.96 O
ATOM	251	CB	ILE	A	33	24.470	55.712	-24.139	1.00	51.31 C
ATOM	252	CG1	ILE	A	33	23.518	56.700	-24.800	1.00	52.96 C
ATOM	253	CG2	ILE	A	33	24.116	55.563	-22.654	1.00	50.09 C
ATOM	254	CD1	ILE	A	33	22.087	56.233	-24.828	1.00	54.31 C
ATOM	255	N	SER	A	34	27.535	55.588	-22.603	1.00	43.80 N
ATOM	256	CA	SER	A	34	28.463	54.716	-21.910	1.00	47.69 C
ATOM	257	C	SER	A	34	28.262	54.831	-20.410	1.00	51.46 C
ATOM	258	O	SER	A	34	27.899	55.892	-19.897	1.00	50.26 O
ATOM	259	CB	SER	A	34	29.898	55.105	-22.255	1.00	44.86 C
ATOM	260	OG	SER	A	34	30.197	54.768	-23.592	1.00	56.99 O
ATOM	261	N	TRP	A	35	28.488	53.726	-19.714	1.00	47.72 N
ATOM	262	CA	TRP	A	35	28.359	53.713	-18.270	1.00	42.75 C
ATOM	263	C	TRP	A	35	29.741	53.598	-17.652	1.00	45.12 C
ATOM	264	O	TRP	A	35	30.640	52.967	-18.223	1.00	44.07 O
ATOM	265	CB	TRP	A	35	27.511	52.531	-17.800	1.00	39.02 C
ATOM	266	CG	TRP	A	35	26.028	52.667	-18.015	1.00	43.96 C
ATOM	267	CD1	TRP	A	35	25.323	52.308	-19.126	1.00	38.82 C
ATOM	268	CD2	TRP	A	35	25.062	53.080	-17.041	1.00	36.18 C
ATOM	269	NE1	TRP	A	35	23.974	52.454	-18.901	1.00	45.99 N
ATOM	270	CE2	TRP	A	35	23.786	52.925	-17.632	1.00	47.03 C
ATOM	271	CE3	TRP	A	35	25.150	53.556	-15.735	1.00	39.81 C
ATOM	272	CZ2	TRP	A	35	22.605	53.232	-16.948	1.00	43.25 C
ATOM	273	CZ3	TRP	A	35	23.962	53.865	-15.054	1.00	41.38 C
ATOM	274	CH2	TRP	A	35	22.713	53.699	-15.668	1.00	42.80 C
ATOM	275	N	PHE	A	36	29.907	54.225	-16.491	1.00	45.19 N
ATOM	276	CA	PHE	A	36	31.160	54.178	-15.748	1.00	44.89 C
ATOM	277	C	PHE	A	36	30.834	53.716	-14.345	1.00	44.82 C
ATOM	278	O	PHE	A	36	29.858	54.166	-13.755	1.00	41.52 O
ATOM	279	CB	PHE	A	36	31.819	55.556	-15.675	1.00	43.10 C
ATOM	280	CG	PHE	A	36	32.286	56.062	-17.006	1.00	55.53 C
ATOM	281	CD1	PHE	A	36	31.385	56.639	-17.893	1.00	51.14 C
ATOM	282	CD2	PHE	A	36	33.610	55.883	-17.407	1.00	46.89 C

Figure 2 (Table 2 (page 13))

ATOM	283	CE1	PHE	A	36	31.789	57.030	-19.173	1.00	54.91	C
ATOM	284	CE2	PHE	A	36	34.030	56.269	-18.684	1.00	55.64	C
ATOM	285	CZ	PHE	A	36	33.110	56.846	-19.573	1.00	50.29	C
ATOM	286	N	SER	A	37	31.641	52.795	-13.832	1.00	42.90	N
ATOM	287	CA	SER	A	37	31.447	52.289	-12.488	1.00	52.59	C
ATOM	288	C	SER	A	37	31.973	53.321	-11.490	1.00	53.66	C
ATOM	289	O	SER	A	37	32.581	54.325	-11.878	1.00	46.56	O
ATOM	290	CB	SER	A	37	32.176	50.950	-12.322	1.00	56.49	C
ATOM	291	OG	SER	A	37	33.540	51.055	-12.675	1.00	54.60	O
ATOM	292	N	PRO	A	38	31.729	53.096	-10.192	1.00	55.82	N
ATOM	293	CA	PRO	A	38	32.169	54.004	-9.124	1.00	58.18	C
ATOM	294	C	PRO	A	38	33.682	54.241	-9.057	1.00	56.07	C
ATOM	295	O	PRO	A	38	34.135	55.248	-8.519	1.00	57.12	O
ATOM	296	CB	PRO	A	38	31.619	53.338	-7.864	1.00	55.81	C
ATOM	297	CG	PRO	A	38	30.327	52.731	-8.377	1.00	51.53	C
ATOM	298	CD	PRO	A	38	30.764	52.107	-9.677	1.00	50.32	C
ATOM	299	N	ASN	A	39	34.456	53.317	-9.609	1.00	52.69	N
ATOM	300	CA	ASN	A	39	35.905	53.452	-9.613	1.00	59.02	C
ATOM	301	C	ASN	A	39	36.396	54.175	-10.881	1.00	61.73	C
ATOM	302	O	ASN	A	39	37.585	54.160	-11.188	1.00	57.13	O
ATOM	303	CB	ASN	A	39	36.551	52.077	-9.523	1.00	56.75	C
ATOM	304	CG	ASN	A	39	36.432	51.310	-10.810	1.00	71.38	C
ATOM	305	OD1	ASN	A	39	35.531	51.565	-11.603	1.00	73.88	O
ATOM	306	ND2	ASN	A	39	37.332	50.361	-11.027	1.00	79.44	N
ATOM	307	N	GLY	A	40	35.471	54.777	-11.626	1.00	54.18	N
ATOM	308	CA	GLY	A	40	35.839	55.523	-12.825	1.00	58.26	C
ATOM	309	C	GLY	A	40	36.049	54.777	-14.126	1.00	56.72	C
ATOM	310	O	GLY	A	40	36.311	55.385	-15.161	1.00	59.14	O
ATOM	311	N	GLU	A	41	35.940	53.462	-14.098	1.00	53.24	N
ATOM	312	CA	GLU	A	41	36.137	52.712	-15.312	1.00	54.15	C
ATOM	313	C	GLU	A	41	34.887	52.572	-16.152	1.00	52.64	C
ATOM	314	O	GLU	A	41	33.772	52.444	-15.645	1.00	51.92	O
ATOM	315	CB	GLU	A	41	36.695	51.341	-14.988	1.00	62.00	C
ATOM	316	CG	GLU	A	41	38.100	51.410	-14.451	1.00	86.56	C
ATOM	317	CD	GLU	A	41	38.565	50.074	-13.931	1.00	94.84	C
ATOM	318	OE1	GLU	A	41	37.901	49.059	-14.243	1.00	99.92	O
ATOM	319	OE2	GLU	A	41	39.591	50.041	-13.220	1.00	98.17	O
ATOM	320	N	LYS	A	42	35.104	52.625	-17.457	1.00	48.52	N
ATOM	321	CA	LYS	A	42	34.050	52.475	-18.430	1.00	45.24	C
ATOM	322	C	LYS	A	42	33.714	50.979	-18.477	1.00	52.84	C
ATOM	323	O	LYS	A	42	34.607	50.126	-18.534	1.00	47.42	O
ATOM	324	CB	LYS	A	42	34.536	52.971	-19.796	1.00	46.19	C
ATOM	325	CG	LYS	A	42	33.502	52.863	-20.930	1.00	58.73	C
ATOM	326	CD	LYS	A	42	34.006	53.553	-22.205	1.00	60.30	C
ATOM	327	CE	LYS	A	42	33.004	53.446	-23.353	1.00	69.24	C
ATOM	328	NZ	LYS	A	42	33.486	54.104	-24.606	1.00	73.95	N
ATOM	329	N	LEU	A	43	32.425	50.659	-18.441	1.00	42.58	N
ATOM	330	CA	LEU	A	43	31.986	49.270	-18.453	1.00	44.33	C
ATOM	331	C	LEU	A	43	31.907	48.724	-19.863	1.00	45.36	C
ATOM	332	O	LEU	A	43	31.315	49.351	-20.734	1.00	49.42	O
ATOM	333	CB	LEU	A	43	30.613	49.177	-17.778	1.00	37.59	C
ATOM	334	CG	LEU	A	43	30.672	49.579	-16.302	1.00	45.02	C
ATOM	335	CD1	LEU	A	43	29.276	49.708	-15.713	1.00	48.59	C
ATOM	336	CD2	LEU	A	43	31.489	48.538	-15.550	1.00	45.09	C
ATOM	337	N	SER	A	44	32.507	47.566	-20.100	0.50	34.43	N
ATOM	338	CA	SER	A	44	32.436	46.990	-21.429	0.50	37.54	C
ATOM	339	C	SER	A	44	31.017	46.509	-21.595	0.50	40.70	C

Figure 2 (Table 2 (page 14))

ATOM	340	O	SER	A	44	30.404	45.984	-20.672	0.50	31.07	O
ATOM	341	CB	SER	A	44	33.394	45.813	-21.590	0.50	34.76	C
ATOM	342	OG	SER	A	44	34.730	46.238	-21.418	0.50	37.63	O
ATOM	343	N	PRO	A	45	30.475	46.684	-22.787	1.00	55.79	N
ATOM	344	CA	PRO	A	45	29.104	46.261	-23.062	1.00	56.53	C
ATOM	345	C	PRO	A	45	28.910	44.761	-23.041	1.00	53.37	C
ATOM	346	O	PRO	A	45	29.849	43.986	-23.229	1.00	56.21	O
ATOM	347	CB	PRO	A	45	28.836	46.833	-24.458	1.00	60.37	C
ATOM	348	CG	PRO	A	45	29.823	47.960	-24.586	1.00	60.02	C
ATOM	349	CD	PRO	A	45	31.056	47.392	-23.941	1.00	63.21	C
ATOM	350	N	ASN	A	46	27.667	44.370	-22.800	1.00	57.48	N
ATOM	351	CA	ASN	A	46	27.279	42.973	-22.812	1.00	57.72	C
ATOM	352	C	ASN	A	46	28.150	41.993	-22.017	1.00	57.75	C
ATOM	353	O	ASN	A	46	28.534	40.950	-22.541	1.00	60.65	O
ATOM	354	CB	ASN	A	46	27.179	42.508	-24.272	1.00	67.80	C
ATOM	355	CG	ASN	A	46	26.285	43.417	-25.119	1.00	71.96	C
ATOM	356	OD1	ASN	A	46	25.090	43.557	-24.850	1.00	81.33	O
ATOM	357	ND2	ASN	A	46	26.862	44.033	-26.146	1.00	70.84	N
ATOM	358	N	GLN	A	47	28.478	42.325	-20.771	1.00	53.34	N
ATOM	359	CA	GLN	A	47	29.250	41.408	-19.925	1.00	49.41	C
ATOM	360	C	GLN	A	47	28.202	40.672	-19.091	1.00	50.32	C
ATOM	361	O	GLN	A	47	27.029	41.040	-19.111	1.00	47.47	O
ATOM	362	CB	GLN	A	47	30.232	42.156	-19.022	1.00	51.46	C
ATOM	363	CG	GLN	A	47	31.291	42.936	-19.798	1.00	49.02	C
ATOM	364	CD	GLN	A	47	32.023	42.055	-20.812	1.00	60.54	C
ATOM	365	OE1	GLN	A	47	32.910	41.286	-20.448	1.00	52.30	O
ATOM	366	NE2	GLN	A	47	31.634	42.149	-22.082	1.00	51.19	N
ATOM	367	N	GLN	A	48	28.630	39.669	-18.336	1.00	52.29	N
ATOM	368	CA	GLN	A	48	27.728	38.807	-17.566	1.00	56.49	C
ATOM	369	C	GLN	A	48	27.049	39.337	-16.305	1.00	58.23	C
ATOM	370	O	GLN	A	48	25.818	39.453	-16.238	1.00	50.89	O
ATOM	371	CB	GLN	A	48	28.486	37.524	-17.199	1.00	69.79	C
ATOM	372	CG	GLN	A	48	27.606	36.324	-16.903	1.00	85.42	C
ATOM	373	CD	GLN	A	48	27.071	35.675	-18.172	1.00	96.52	C
ATOM	374	OE1	GLN	A	48	27.848	35.302	-19.052	1.00	103.65	O
ATOM	375	NE2	GLN	A	48	25.745	35.530	-18.272	1.00	97.26	N
ATOM	376	N	ARG	A	49	27.866	39.613	-15.297	1.00	46.27	N
ATOM	377	CA	ARG	A	49	27.376	40.069	-14.009	1.00	49.02	C
ATOM	378	C	ARG	A	49	27.031	41.558	-13.965	1.00	50.34	C
ATOM	379	O	ARG	A	49	25.951	41.929	-13.518	1.00	44.46	O
ATOM	380	CB	ARG	A	49	28.404	39.724	-12.937	1.00	43.05	C
ATOM	381	CG	ARG	A	49	27.841	39.691	-11.541	1.00	50.00	C
ATOM	382	CD	ARG	A	49	28.920	39.301	-10.560	1.00	46.14	C
ATOM	383	NE	ARG	A	49	29.847	40.402	-10.332	1.00	50.29	N
ATOM	384	CZ	ARG	A	49	29.552	41.479	-9.614	1.00	49.75	C
ATOM	385	NH1	ARG	A	49	28.355	41.602	-9.054	1.00	46.61	N
ATOM	386	NH2	ARG	A	49	30.456	42.434	-9.450	1.00	54.16	N
ATOM	387	N	ILE	A	50	27.950	42.413	-14.404	1.00	45.13	N
ATOM	388	CA	ILE	A	50	27.693	43.846	-14.431	1.00	47.45	C
ATOM	389	C	ILE	A	50	27.362	44.081	-15.886	1.00	49.10	C
ATOM	390	O	ILE	A	50	28.236	44.288	-16.718	1.00	46.05	O
ATOM	391	CB	ILE	A	50	28.927	44.633	-13.989	1.00	46.67	C
ATOM	392	CG1	ILE	A	50	29.309	44.197	-12.569	1.00	49.39	C
ATOM	393	CG2	ILE	A	50	28.645	46.122	-14.047	1.00	45.96	C
ATOM	394	CD1	ILE	A	50	28.175	44.305	-11.547	1.00	38.44	C
ATOM	395	N	SER	A	51	26.069	44.019	-16.172	1.00	45.97	N
ATOM	396	CA	SER	A	51	25.572	44.111	-17.523	1.00	42.85	C

Figure 2 (Table 2 (page 15))

ATOM	397	C	SER	A	51	25.123	45.464	-18.027	1.00	47.59	C
ATOM	398	O	SER	A	51	24.300	46.145	-17.408	1.00	47.20	O
ATOM	399	CB	SER	A	51	24.430	43.096	-17.676	1.00	42.67	C
ATOM	400	OG	SER	A	51	23.643	43.375	-18.811	1.00	55.89	O
ATOM	401	N	VAL	A	52	25.689	45.856	-19.159	1.00	45.49	N
ATOM	402	CA	VAL	A	52	25.317	47.100	-19.802	1.00	46.68	C
ATOM	403	C	VAL	A	52	24.768	46.706	-21.155	1.00	52.16	C
ATOM	404	O	VAL	A	52	25.483	46.140	-21.991	1.00	52.43	O
ATOM	405	CB	VAL	A	52	26.504	48.038	-20.028	1.00	51.87	C
ATOM	406	CG1	VAL	A	52	26.064	49.202	-20.901	1.00	49.68	C
ATOM	407	CG2	VAL	A	52	27.029	48.555	-18.694	1.00	46.22	C
ATOM	408	N	VAL	A	53	23.491	46.999	-21.353	1.00	43.80	N
ATOM	409	CA	VAL	A	53	22.813	46.679	-22.584	1.00	51.71	C
ATOM	410	C	VAL	A	53	22.126	47.901	-23.192	1.00	60.49	C
ATOM	411	O	VAL	A	53	21.288	48.550	-22.564	1.00	55.82	O
ATOM	412	CB	VAL	A	53	21.770	45.573	-22.343	1.00	57.05	C
ATOM	413	CG1	VAL	A	53	20.897	45.392	-23.569	1.00	61.58	C
ATOM	414	CG2	VAL	A	53	22.478	44.269	-22.008	1.00	51.45	C
ATOM	415	N	TRP	A	54	22.511	48.205	-24.422	1.00	65.48	N
ATOM	416	CA	TRP	A	54	21.948	49.309	-25.178	1.00	74.11	C
ATOM	417	C	TRP	A	54	20.581	48.813	-25.650	1.00	74.48	C
ATOM	418	O	TRP	A	54	20.475	47.706	-26.167	1.00	72.95	O
ATOM	419	CB	TRP	A	54	22.851	49.571	-26.365	1.00	82.17	C
ATOM	420	CG	TRP	A	54	22.565	50.791	-27.135	1.00	99.79	C
ATOM	421	CD1	TRP	A	54	22.877	52.073	-26.787	1.00	102.50	C
ATOM	422	CD2	TRP	A	54	22.021	50.849	-28.456	1.00	107.53	C
ATOM	423	NE1	TRP	A	54	22.573	52.929	-27.817	1.00	109.34	N
ATOM	424	CE2	TRP	A	54	22.045	52.205	-28.852	1.00	111.35	C
ATOM	425	CE3	TRP	A	54	21.515	49.889	-29.343	1.00	108.73	C
ATOM	426	CZ2	TRP	A	54	21.590	52.619	-30.108	1.00	112.86	C
ATOM	427	CZ3	TRP	A	54	21.061	50.305	-30.591	1.00	109.55	C
ATOM	428	CH2	TRP	A	54	21.100	51.662	-30.959	1.00	110.38	C
ATOM	429	N	ASN	A	55	19.537	49.612	-25.471	1.00	71.63	N
ATOM	430	CA	ASN	A	55	18.205	49.185	-25.878	1.00	76.76	C
ATOM	431	C	ASN	A	55	17.845	49.651	-27.281	1.00	81.91	C
ATOM	432	O	ASN	A	55	17.573	48.846	-28.168	1.00	88.33	O
ATOM	433	CB	ASN	A	55	17.197	49.689	-24.858	1.00	71.55	C
ATOM	434	CG	ASN	A	55	17.474	49.141	-23.476	1.00	75.04	C
ATOM	435	OD1	ASN	A	55	17.374	47.932	-23.246	1.00	72.25	O
ATOM	436	ND2	ASN	A	55	17.841	50.021	-22.550	1.00	50.95	N
ATOM	437	N	ASP	A	56	17.833	50.962	-27.455	1.00	88.42	N
ATOM	438	CA	ASP	A	56	17.548	51.607	-28.722	1.00	96.25	C
ATOM	439	C	ASP	A	56	18.566	52.727	-28.677	1.00	101.81	C
ATOM	440	O	ASP	A	56	19.369	52.797	-27.736	1.00	102.77	O
ATOM	441	CB	ASP	A	56	16.107	52.147	-28.744	1.00	95.48	C
ATOM	442	CG	ASP	A	56	15.707	52.811	-27.433	1.00	93.76	C
ATOM	443	OD1	ASP	A	56	16.451	53.704	-26.985	1.00	85.05	O
ATOM	444	OD2	ASP	A	56	14.658	52.452	-26.849	1.00	93.98	O
ATOM	445	N	ASP	A	57	18.599	53.607	-29.663	1.00	102.50	N
ATOM	446	CA	ASP	A	57	19.610	54.674	-29.562	1.00	102.11	C
ATOM	447	C	ASP	A	57	19.218	55.678	-28.491	1.00	97.41	C
ATOM	448	O	ASP	A	57	19.933	56.652	-28.258	1.00	97.40	O
ATOM	449	CB	ASP	A	57	19.781	55.395	-30.900	1.00	112.19	C
ATOM	450	CG	ASP	A	57	21.068	56.116	-30.995	1.00	121.70	C
ATOM	451	OD1	ASP	A	57	21.660	56.543	-29.959	1.00	128.34	O
ATOM	452	OD2	ASP	A	57	21.589	56.364	-32.125	1.00	123.94	O
ATOM	453	N	ASP	A	58	18.084	55.433	-27.843	1.00	90.49	N



Figure 2 (Table 2 (page 16))

ATOM	454	CA	ASP	A	58	17.622	56.352	-26.826	1.00	87.06	C
ATOM	455	C	ASP	A	58	18.071	55.997	-25.427	1.00	73.82	C
ATOM	456	O	ASP	A	58	18.180	56.880	-24.577	1.00	62.84	O
ATOM	457	CB	ASP	A	58	16.093	56.433	-26.809	1.00	103.58	C
ATOM	458	CG	ASP	A	58	15.487	56.564	-28.191	1.00	113.84	C
ATOM	459	OD1	ASP	A	58	15.498	57.677	-28.763	1.00	117.69	O
ATOM	460	OD2	ASP	A	58	14.997	55.534	-28.700	1.00	121.72	O
ATOM	461	N	SER	A	59	18.320	54.717	-25.174	1.00	64.75	N
ATOM	462	CA	SER	A	59	18.681	54.313	-23.828	1.00	61.90	C
ATOM	463	C	SER	A	59	19.628	53.131	-23.689	1.00	64.15	C
ATOM	464	O	SER	A	59	19.869	52.359	-24.627	1.00	60.43	O
ATOM	465	CB	SER	A	59	17.408	54.000	-23.052	1.00	55.02	C
ATOM	466	OG	SER	A	59	16.760	52.881	-23.625	1.00	62.54	O
ATOM	467	N	SER	A	60	20.145	53.005	-22.473	1.00	58.32	N
ATOM	468	CA	SER	A	60	21.062	51.941	-22.111	1.00	53.12	C
ATOM	469	C	SER	A	60	20.694	51.465	-20.708	1.00	51.38	C
ATOM	470	O	SER	A	60	20.439	52.271	-19.815	1.00	50.11	O
ATOM	471	CB	SER	A	60	22.502	52.451	-22.127	1.00	48.06	C
ATOM	472	OG	SER	A	60	23.407	51.420	-21.751	1.00	54.93	O
ATOM	473	N	THR	A	61	20.667	50.157	-20.509	1.00	41.41	N
ATOM	474	CA	THR	A	61	20.308	49.618	-19.206	1.00	44.19	C
ATOM	475	C	THR	A	61	21.489	48.979	-18.501	1.00	42.41	C
ATOM	476	O	THR	A	61	22.227	48.188	-19.081	1.00	46.93	O
ATOM	477	CB	THR	A	61	19.183	48.583	-19.353	1.00	47.49	C
ATOM	478	OG1	THR	A	61	18.023	49.233	-19.880	1.00	56.06	O
ATOM	479	CG2	THR	A	61	18.837	47.945	-18.004	1.00	45.18	C
ATOM	480	N	LEU	A	62	21.674	49.359	-17.247	1.00	37.61	N
ATOM	481	CA	LEU	A	62	22.731	48.797	-16.432	1.00	39.04	C
ATOM	482	C	LEU	A	62	22.076	47.810	-15.475	1.00	38.19	C
ATOM	483	O	LEU	A	62	21.171	48.185	-14.722	1.00	38.43	O
ATOM	484	CB	LEU	A	62	23.431	49.896	-15.628	1.00	34.82	C
ATOM	485	CG	LEU	A	62	24.273	49.373	-14.461	1.00	46.86	C
ATOM	486	CD1	LEU	A	62	25.418	48.550	-14.996	1.00	41.11	C
ATOM	487	CD2	LEU	A	62	24.797	50.517	-13.617	1.00	40.98	C
ATOM	488	N	THR	A	63	22.488	46.548	-15.514	1.00	34.32	N
ATOM	489	CA	THR	A	63	21.930	45.570	-14.583	1.00	42.11	C
ATOM	490	C	THR	A	63	23.043	45.058	-13.694	1.00	38.02	C
ATOM	491	O	THR	A	63	24.086	44.634	-14.181	1.00	39.91	O
ATOM	492	CB	THR	A	63	21.312	44.333	-15.284	1.00	44.60	C
ATOM	493	OG1	THR	A	63	20.291	44.746	-16.193	1.00	38.13	O
ATOM	494	CG2	THR	A	63	20.709	43.388	-14.247	1.00	41.53	C
ATOM	495	N	ILE	A	64	22.831	45.096	-12.390	1.00	32.30	N
ATOM	496	CA	ILE	A	64	23.835	44.596	-11.464	1.00	40.27	C
ATOM	497	C	ILE	A	64	23.288	43.299	-10.884	1.00	44.61	C
ATOM	498	O	ILE	A	64	22.400	43.324	-10.032	1.00	43.38	O
ATOM	499	CB	ILE	A	64	24.116	45.600	-10.319	1.00	43.07	C
ATOM	500	CG1	ILE	A	64	24.757	46.868	-10.894	1.00	50.00	C
ATOM	501	CG2	ILE	A	64	25.032	44.962	-9.265	1.00	36.35	C
ATOM	502	CD1	ILE	A	64	25.080	47.930	-9.867	1.00	45.66	C
ATOM	503	N	TYR	A	65	23.811	42.175	-11.373	1.00	41.50	N
ATOM	504	CA	TYR	A	65	23.398	40.851	-10.917	1.00	41.75	C
ATOM	505	C	TYR	A	65	24.239	40.399	-9.746	1.00	46.17	C
ATOM	506	O	TYR	A	65	25.400	40.796	-9.628	1.00	46.44	O
ATOM	507	CB	TYR	A	65	23.591	39.814	-12.023	1.00	39.24	C
ATOM	508	CG	TYR	A	65	22.643	39.936	-13.177	1.00	46.02	C
ATOM	509	CD1	TYR	A	65	23.074	40.408	-14.415	1.00	43.20	C
ATOM	510	CD2	TYR	A	65	21.304	39.560	-13.035	1.00	40.19	C

Figure 2 (Table 2 (page 17))

ATOM	511	CE1	TYR	A	65	22.198	40.503	-15.492	1.00	46.92	C
ATOM	512	CE2	TYR	A	65	20.406	39.644	-14.117	1.00	42.02	C
ATOM	513	CZ	TYR	A	65	20.868	40.117	-15.337	1.00	47.29	C
ATOM	514	OH	TYR	A	65	20.008	40.185	-16.399	1.00	46.88	O
ATOM	515	N	ASN	A	66	23.660	39.556	-8.897	1.00	43.81	N
ATOM	516	CA	ASN	A	66	24.368	38.990	-7.756	1.00	48.17	C
ATOM	517	C	ASN	A	66	25.277	40.002	-7.062	1.00	48.24	C
ATOM	518	O	ASN	A	66	26.489	39.792	-6.955	1.00	48.04	O
ATOM	519	CB	ASN	A	66	25.206	37.817	-8.241	1.00	44.79	C
ATOM	520	CG	ASN	A	66	25.844	37.052	-7.100	1.00	58.80	C
ATOM	521	OD1	ASN	A	66	26.868	36.393	-7.279	1.00	62.64	O
ATOM	522	ND2	ASN	A	66	25.237	37.127	-5.919	1.00	60.17	N
ATOM	523	N	ALA	A	67	24.684	41.080	-6.566	1.00	47.68	N
ATOM	524	CA	ALA	A	67	25.448	42.151	-5.935	1.00	40.81	C
ATOM	525	C	ALA	A	67	26.301	41.798	-4.739	1.00	49.08	C
ATOM	526	O	ALA	A	67	25.937	40.963	-3.910	1.00	47.57	O
ATOM	527	CB	ALA	A	67	24.523	43.290	-5.553	1.00	44.48	C
ATOM	528	N	ASN	A	68	27.435	42.482	-4.649	1.00	50.95	N
ATOM	529	CA	ASN	A	68	28.344	42.315	-3.529	1.00	54.43	C
ATOM	530	C	ASN	A	68	28.763	43.719	-3.093	1.00	55.80	C
ATOM	531	O	ASN	A	68	28.665	44.678	-3.872	1.00	45.45	O
ATOM	532	CB	ASN	A	68	29.557	41.476	-3.922	1.00	51.73	C
ATOM	533	CG	ASN	A	68	30.494	42.201	-4.854	1.00	61.49	C
ATOM	534	OD1	ASN	A	68	30.920	43.322	-4.579	1.00	60.88	O
ATOM	535	ND2	ASN	A	68	30.835	41.554	-5.963	1.00	52.62	N
ATOM	536	N	ILE	A	69	29.235	43.835	-1.856	1.00	52.73	N
ATOM	537	CA	ILE	A	69	29.630	45.118	-1.285	1.00	58.71	C
ATOM	538	C	ILE	A	69	30.545	45.990	-2.137	1.00	51.79	C
ATOM	539	O	ILE	A	69	30.483	47.208	-2.043	1.00	52.79	O
ATOM	540	CB	ILE	A	69	30.299	44.937	0.095	1.00	60.50	C
ATOM	541	CG1	ILE	A	69	31.681	44.301	-0.063	1.00	67.17	C
ATOM	542	CG2	ILE	A	69	29.410	44.091	0.987	1.00	59.59	C
ATOM	543	CD1	ILE	A	69	32.506	44.314	1.211	1.00	80.29	C
ATOM	544	N	ASP	A	70	31.396	45.384	-2.956	1.00	46.36	N
ATOM	545	CA	ASP	A	70	32.277	46.184	-3.781	1.00	50.45	C
ATOM	546	C	ASP	A	70	31.587	46.792	-4.991	1.00	58.77	C
ATOM	547	O	ASP	A	70	32.227	47.477	-5.784	1.00	53.61	O
ATOM	548	CB	ASP	A	70	33.473	45.369	-4.241	1.00	50.41	C
ATOM	549	CG	ASP	A	70	34.388	44.991	-3.088	1.00	69.82	C
ATOM	550	OD1	ASP	A	70	34.622	45.851	-2.208	1.00	68.65	O
ATOM	551	OD2	ASP	A	70	34.878	43.842	-3.064	1.00	67.67	O
ATOM	552	N	ASP	A	71	30.290	46.540	-5.144	1.00	54.09	N
ATOM	553	CA	ASP	A	71	29.554	47.102	-6.269	1.00	50.10	C
ATOM	554	C	ASP	A	71	28.969	48.474	-5.898	1.00	52.41	C
ATOM	555	O	ASP	A	71	28.508	49.224	-6.764	1.00	47.41	O
ATOM	556	CB	ASP	A	71	28.406	46.166	-6.708	1.00	49.99	C
ATOM	557	CG	ASP	A	71	28.892	44.834	-7.302	1.00	49.02	C
ATOM	558	OD1	ASP	A	71	29.813	44.825	-8.146	1.00	46.46	O
ATOM	559	OD2	ASP	A	71	28.324	43.784	-6.929	1.00	50.74	O
ATOM	560	N	ALA	A	72	28.987	48.801	-4.610	1.00	42.72	N
ATOM	561	CA	ALA	A	72	28.429	50.063	-4.133	1.00	45.31	C
ATOM	562	C	ALA	A	72	29.129	51.291	-4.686	1.00	47.73	C
ATOM	563	O	ALA	A	72	30.326	51.268	-4.977	1.00	47.41	O
ATOM	564	CB	ALA	A	72	28.460	50.107	-2.604	1.00	47.05	C
ATOM	565	N	GLY	A	73	28.378	52.374	-4.821	1.00	48.72	N
ATOM	566	CA	GLY	A	73	28.976	53.593	-5.322	1.00	54.09	C
ATOM	567	C	GLY	A	73	28.144	54.331	-6.341	1.00	51.98	C

Figure 2 (Table 2 (page 18))

ATOM	568	O	GLY	A	73	27.018	53.939	-6.653	1.00	49.57	O
ATOM	569	N	ILE	A	74	28.716	55.413	-6.859	1.00	51.79	N
ATOM	570	CA	ILE	A	74	28.052	56.242	-7.850	1.00	48.58	C
ATOM	571	C	ILE	A	74	28.428	55.760	-9.237	1.00	47.75	C
ATOM	572	O	ILE	A	74	29.603	55.780	-9.620	1.00	46.87	O
ATOM	573	CB	ILE	A	74	28.475	57.717	-7.705	1.00	54.10	C
ATOM	574	CG1	ILE	A	74	28.061	58.227	-6.323	1.00	60.29	C
ATOM	575	CG2	ILE	A	74	27.860	58.551	-8.816	1.00	51.72	C
ATOM	576	CD1	ILE	A	74	28.463	59.656	-6.041	1.00	55.15	C
ATOM	577	N	TYR	A	75	27.429	55.272	-9.960	1.00	39.87	N
ATOM	578	CA	TYR	A	75	27.637	54.826	-11.330	1.00	48.23	C
ATOM	579	C	TYR	A	75	27.168	56.010	-12.126	1.00	48.15	C
ATOM	580	O	TYR	A	75	26.293	56.764	-11.682	1.00	46.43	O
ATOM	581	CB	TYR	A	75	26.745	53.629	-11.707	1.00	44.56	C
ATOM	582	CG	TYR	A	75	27.137	52.331	-11.050	1.00	47.56	C
ATOM	583	CD1	TYR	A	75	26.925	52.133	-9.682	1.00	39.03	C
ATOM	584	CD2	TYR	A	75	27.789	51.326	-11.773	1.00	43.44	C
ATOM	585	CE1	TYR	A	75	27.356	50.967	-9.045	1.00	39.99	C
ATOM	586	CE2	TYR	A	75	28.230	50.162	-11.146	1.00	32.79	C
ATOM	587	CZ	TYR	A	75	28.010	49.990	-9.778	1.00	35.84	C
ATOM	588	OH	TYR	A	75	28.463	48.851	-9.153	1.00	43.95	O
ATOM	589	N	LYS	A	76	27.739	56.201	-13.299	1.00	48.85	N
ATOM	590	CA	LYS	A	76	27.270	57.305	-14.090	1.00	48.84	C
ATOM	591	C	LYS	A	76	27.178	56.938	-15.532	1.00	44.98	C
ATOM	592	O	LYS	A	76	27.912	56.092	-16.052	1.00	47.18	O
ATOM	593	CB	LYS	A	76	28.115	58.551	-13.857	1.00	56.56	C
ATOM	594	CG	LYS	A	76	29.442	58.619	-14.520	1.00	59.09	C
ATOM	595	CD	LYS	A	76	30.046	59.941	-14.072	1.00	66.83	C
ATOM	596	CE	LYS	A	76	31.142	60.452	-14.968	1.00	71.43	C
ATOM	597	NZ	LYS	A	76	31.553	61.794	-14.449	1.00	73.15	N
ATOM	598	N	CYS	A	77	26.194	57.553	-16.153	1.00	45.89	N
ATOM	599	CA	CYS	A	77	25.888	57.319	-17.532	1.00	44.65	C
ATOM	600	C	CYS	A	77	26.233	58.600	-18.270	1.00	47.89	C
ATOM	601	O	CYS	A	77	25.718	59.666	-17.945	1.00	52.98	O
ATOM	602	CB	CYS	A	77	24.401	57.004	-17.652	1.00	42.61	C
ATOM	603	SG	CYS	A	77	23.808	56.802	-19.350	1.00	61.23	S
ATOM	604	N	VAL	A	78	27.122	58.494	-19.249	1.00	50.12	N
ATOM	605	CA	VAL	A	78	27.547	59.658	-20.019	1.00	46.50	C
ATOM	606	C	VAL	A	78	27.082	59.581	-21.471	1.00	43.99	C
ATOM	607	O	VAL	A	78	27.222	58.552	-22.131	1.00	48.45	O
ATOM	608	CB	VAL	A	78	29.084	59.795	-19.993	1.00	46.58	C
ATOM	609	CG1	VAL	A	78	29.517	61.010	-20.820	1.00	51.99	C
ATOM	610	CG2	VAL	A	78	29.566	59.942	-18.547	1.00	41.06	C
ATOM	611	N	VAL	A	79	26.521	60.672	-21.965	1.00	48.68	N
ATOM	612	CA	VAL	A	79	26.047	60.720	-23.343	1.00	57.39	C
ATOM	613	C	VAL	A	79	26.945	61.666	-24.119	1.00	54.87	C
ATOM	614	O	VAL	A	79	27.194	62.792	-23.691	1.00	52.91	O
ATOM	615	CB	VAL	A	79	24.598	61.227	-23.417	1.00	60.20	C
ATOM	616	CG1	VAL	A	79	24.085	61.155	-24.848	1.00	54.06	C
ATOM	617	CG2	VAL	A	79	23.730	60.395	-22.487	1.00	56.02	C
ATOM	618	N	THR	A	80	27.452	61.191	-25.247	1.00	48.32	N
ATOM	619	CA	THR	A	80	28.313	62.011	-26.066	1.00	52.81	C
ATOM	620	C	THR	A	80	27.706	62.226	-27.450	1.00	54.17	C
ATOM	621	O	THR	A	80	27.501	61.266	-28.187	1.00	49.22	O
ATOM	622	CB	THR	A	80	29.691	61.371	-26.241	1.00	54.94	C
ATOM	623	OG1	THR	A	80	30.268	61.104	-24.954	1.00	54.31	O
ATOM	624	CG2	THR	A	80	30.601	62.318	-27.012	1.00	41.33	C

Figure 2 (Table 2 (page 19))

ATOM	625	N	ALA	A	81	27.430	63.487	-27.787	1.00	56.76	N
ATOM	626	CA	ALA	A	81	26.859	63.866	-29.088	1.00	58.85	C
ATOM	627	C	ALA	A	81	27.942	63.828	-30.165	1.00	58.97	C
ATOM	628	O	ALA	A	81	29.131	63.922	-29.847	1.00	53.72	O
ATOM	629	CB	ALA	A	81	26.263	65.265	-29.005	1.00	60.88	C
ATOM	630	N	GLU	A	82	27.528	63.712	-31.429	1.00	67.86	N
ATOM	631	CA	GLU	A	82	28.462	63.639	-32.555	1.00	73.18	C
ATOM	632	C	GLU	A	82	29.599	64.664	-32.507	1.00	68.06	C
ATOM	633	O	GLU	A	82	30.700	64.398	-32.993	1.00	65.36	O
ATOM	634	CB	GLU	A	82	27.707	63.768	-33.887	1.00	74.95	C
ATOM	635	CG	GLU	A	82	28.027	62.638	-34.868	1.00	98.35	C
ATOM	636	CD	GLU	A	82	27.295	62.768	-36.194	1.00	111.66	C
ATOM	637	OE1	GLU	A	82	26.071	63.034	-36.178	1.00	118.11	O
ATOM	638	OE2	GLU	A	82	27.942	62.594	-37.253	1.00	117.01	O
ATOM	639	N	ASP	A	83	29.340	65.821	-31.907	1.00	62.35	N
ATOM	640	CA	ASP	A	83	30.340	66.877	-31.812	1.00	67.89	C
ATOM	641	C	ASP	A	83	31.171	66.830	-30.533	1.00	71.00	C
ATOM	642	O	ASP	A	83	31.929	67.759	-30.246	1.00	73.73	O
ATOM	643	CB	ASP	A	83	29.653	68.230	-31.924	1.00	74.31	C
ATOM	644	CG	ASP	A	83	28.664	68.461	-30.815	1.00	82.18	C
ATOM	645	OD1	ASP	A	83	27.939	67.508	-30.462	1.00	93.75	O
ATOM	646	OD2	ASP	A	83	28.606	69.593	-30.301	1.00	87.77	O
ATOM	647	N	GLY	A	84	31.017	65.760	-29.759	1.00	69.26	N
ATOM	648	CA	GLY	A	84	31.790	65.617	-28.533	1.00	61.95	C
ATOM	649	C	GLY	A	84	31.242	66.254	-27.266	1.00	62.86	C
ATOM	650	O	GLY	A	84	31.851	66.139	-26.197	1.00	65.82	O
ATOM	651	N	THR	A	85	30.106	66.936	-27.361	1.00	55.77	N
ATOM	652	CA	THR	A	85	29.535	67.559	-26.176	1.00	63.65	C
ATOM	653	C	THR	A	85	28.929	66.445	-25.320	1.00	61.95	C
ATOM	654	O	THR	A	85	28.291	65.528	-25.839	1.00	56.86	O
ATOM	655	CB	THR	A	85	28.471	68.614	-26.555	1.00	61.72	C
ATOM	656	OG1	THR	A	85	27.458	68.019	-27.373	1.00	73.83	O
ATOM	657	CG2	THR	A	85	29.125	69.749	-27.325	1.00	69.89	C
ATOM	658	N	GLN	A	86	29.130	66.520	-24.011	1.00	58.16	N
ATOM	659	CA	GLN	A	86	28.628	65.464	-23.141	1.00	63.76	C
ATOM	660	C	GLN	A	86	27.696	65.900	-22.030	1.00	62.47	C
ATOM	661	O	GLN	A	86	27.803	67.011	-21.505	1.00	64.92	O
ATOM	662	CB	GLN	A	86	29.793	64.715	-22.498	1.00	56.96	C
ATOM	663	CG	GLN	A	86	30.860	64.242	-23.460	1.00	50.20	C
ATOM	664	CD	GLN	A	86	31.964	63.519	-22.724	1.00	54.10	C
ATOM	665	OE1	GLN	A	86	32.390	63.965	-21.663	1.00	54.08	O
ATOM	666	NE2	GLN	A	86	32.436	62.401	-23.276	1.00	56.27	N
ATOM	667	N	SER	A	87	26.800	64.986	-21.667	1.00	63.47	N
ATOM	668	CA	SER	A	87	25.836	65.182	-20.588	1.00	68.11	C
ATOM	669	C	SER	A	87	25.889	63.906	-19.749	1.00	65.62	C
ATOM	670	O	SER	A	87	26.194	62.829	-20.270	1.00	69.37	O
ATOM	671	CB	SER	A	87	24.420	65.362	-21.150	1.00	75.52	C
ATOM	672	OG	SER	A	87	24.344	66.449	-22.057	1.00	88.36	O
ATOM	673	N	GLU	A	88	25.592	64.009	-18.460	1.00	63.19	N
ATOM	674	CA	GLU	A	88	25.623	62.827	-17.607	1.00	53.44	C
ATOM	675	C	GLU	A	88	24.532	62.803	-16.556	1.00	59.13	C
ATOM	676	O	GLU	A	88	23.942	63.824	-16.209	1.00	58.88	O
ATOM	677	CB	GLU	A	88	26.976	62.711	-16.904	1.00	60.59	C
ATOM	678	CG	GLU	A	88	27.272	63.816	-15.898	1.00	67.25	C
ATOM	679	CD	GLU	A	88	28.656	63.687	-15.277	1.00	78.40	C
ATOM	680	OE1	GLU	A	88	29.631	63.494	-16.035	1.00	79.36	O
ATOM	681	OE2	GLU	A	88	28.773	63.782	-14.033	1.00	81.96	O

Figure 2 (Table 2 (page 20))

ATOM	682	N	ALA	A	89	24.254	61.602	-16.079	1.00	54.88	N
ATOM	683	CA	ALA	A	89	23.283	61.384	-15.027	1.00	45.50	C
ATOM	684	C	ALA	A	89	24.036	60.407	-14.149	1.00	52.74	C
ATOM	685	O	ALA	A	89	24.777	59.552	-14.659	1.00	48.26	O
ATOM	686	CB	ALA	A	89	22.022	60.736	-15.567	1.00	53.66	C
ATOM	687	N	THR	A	90	23.887	60.549	-12.839	1.00	46.21	N
ATOM	688	CA	THR	A	90	24.558	59.647	-11.932	1.00	49.08	C
ATOM	689	C	THR	A	90	23.515	58.993	-11.051	1.00	49.13	C
ATOM	690	O	THR	A	90	22.402	59.516	-10.861	1.00	49.24	O
ATOM	691	CB	THR	A	90	25.587	60.376	-11.052	1.00	48.30	C
ATOM	692	OG1	THR	A	90	24.932	61.366	-10.256	1.00	53.97	O
ATOM	693	CG2	THR	A	90	26.640	61.041	-11.915	1.00	52.65	C
ATOM	694	N	VAL	A	91	23.871	57.823	-10.539	1.00	45.14	N
ATOM	695	CA	VAL	A	91	22.966	57.102	-9.667	1.00	48.65	C
ATOM	696	C	VAL	A	91	23.736	56.474	-8.527	1.00	45.53	C
ATOM	697	O	VAL	A	91	24.708	55.754	-8.740	1.00	47.93	O
ATOM	698	CB	VAL	A	91	22.164	56.035	-10.433	1.00	50.62	C
ATOM	699	CG1	VAL	A	91	23.113	55.013	-11.094	1.00	48.35	C
ATOM	700	CG2	VAL	A	91	21.177	55.349	-9.474	1.00	54.01	C
ATOM	701	N	ASN	A	92	23.304	56.773	-7.306	1.00	49.96	N
ATOM	702	CA	ASN	A	92	23.964	56.255	-6.116	1.00	50.90	C
ATOM	703	C	ASN	A	92	23.399	54.887	-5.780	1.00	45.05	C
ATOM	704	O	ASN	A	92	22.220	54.742	-5.466	1.00	48.81	O
ATOM	705	CB	ASN	A	92	23.757	57.200	-4.932	1.00	47.93	C
ATOM	706	CG	ASN	A	92	24.569	56.786	-3.724	1.00	54.25	C
ATOM	707	OD1	ASN	A	92	24.115	56.897	-2.584	1.00	56.44	O
ATOM	708	ND2	ASN	A	92	25.784	56.304	-3.969	1.00	54.09	N
ATOM	709	N	VAL	A	93	24.256	53.881	-5.851	1.00	46.44	N
ATOM	710	CA	VAL	A	93	23.831	52.527	-5.574	1.00	47.68	C
ATOM	711	C	VAL	A	93	24.387	52.085	-4.232	1.00	46.87	C
ATOM	712	O	VAL	A	93	25.602	52.009	-4.053	1.00	45.39	O
ATOM	713	CB	VAL	A	93	24.310	51.548	-6.679	1.00	44.88	C
ATOM	714	CG1	VAL	A	93	23.834	50.143	-6.365	1.00	50.34	C
ATOM	715	CG2	VAL	A	93	23.769	51.981	-8.042	1.00	51.13	C
ATOM	716	N	LYS	A	94	23.490	51.807	-3.290	1.00	52.11	N
ATOM	717	CA	LYS	A	94	23.902	51.347	-1.961	1.00	59.43	C
ATOM	718	C	LYS	A	94	23.774	49.832	-1.886	1.00	55.63	C
ATOM	719	O	LYS	A	94	22.871	49.241	-2.471	1.00	43.24	O
ATOM	720	CB	LYS	A	94	23.033	51.960	-0.855	1.00	55.35	C
ATOM	721	CG	LYS	A	94	23.173	53.464	-0.668	1.00	65.17	C
ATOM	722	CD	LYS	A	94	22.156	53.977	0.356	1.00	67.48	C
ATOM	723	CE	LYS	A	94	22.081	55.492	0.362	1.00	74.84	C
ATOM	724	NZ	LYS	A	94	21.040	55.986	1.310	1.00	78.54	N
ATOM	725	N	ILE	A	95	24.699	49.202	-1.181	1.00	56.66	N
ATOM	726	CA	ILE	A	95	24.658	47.762	-1.004	1.00	56.71	C
ATOM	727	C	ILE	A	95	24.467	47.546	0.495	1.00	59.65	C
ATOM	728	O	ILE	A	95	25.004	48.298	1.305	1.00	53.96	O
ATOM	729	CB	ILE	A	95	25.981	47.086	-1.451	1.00	50.11	C
ATOM	730	CG1	ILE	A	95	26.247	47.361	-2.935	1.00	58.21	C
ATOM	731	CG2	ILE	A	95	25.905	45.584	-1.206	1.00	55.81	C
ATOM	732	CD1	ILE	A	95	25.141	46.878	-3.869	1.00	46.59	C
ATOM	733	N	PHE	A	96	23.670	46.553	0.863	1.00	56.77	N
ATOM	734	CA	PHE	A	96	23.464	46.249	2.269	1.00	56.57	C
ATOM	735	C	PHE	A	96	23.070	44.791	2.380	1.00	52.33	C
ATOM	736	O	PHE	A	96	22.921	44.087	1.375	1.00	55.58	O
ATOM	737	CB	PHE	A	96	22.389	47.146	2.893	1.00	51.68	C

Figure 2 (Table 2 (page 21))

ATOM	738	CG	PHE	A	96	20.984	46.731	2.570	1.00	55.80	C
ATOM	739	CD1	PHE	A	96	20.078	46.441	3.589	1.00	56.18	C
ATOM	740	CD2	PHE	A	96	20.565	46.630	1.249	1.00	53.68	C
ATOM	741	CE1	PHE	A	96	18.770	46.055	3.287	1.00	61.36	C
ATOM	742	CE2	PHE	A	96	19.268	46.249	0.932	1.00	54.41	C
ATOM	743	CZ	PHE	A	96	18.362	45.959	1.951	1.00	51.56	C
ATOM	744	N	GLN	A	97	22.929	44.323	3.607	1.00	44.80	N
ATOM	745	CA	GLN	A	97	22.565	42.945	3.819	1.00	41.35	C
ATOM	746	C	GLN	A	97	21.257	42.956	4.559	1.00	43.49	C
ATOM	747	O	GLN	A	97	21.185	43.352	5.725	1.00	48.61	O
ATOM	748	CB	GLN	A	97	23.639	42.220	4.639	1.00	50.03	C
ATOM	749	CG	GLN	A	97	23.239	40.811	5.074	1.00	42.38	C
ATOM	750	CD	GLN	A	97	22.968	39.885	3.899	1.00	45.87	C
ATOM	751	OE1	GLN	A	97	23.879	39.539	3.148	1.00	50.97	O
ATOM	752	NE2	GLN	A	97	21.712	39.485	3.725	1.00	43.50	N
ATOM	753	N	LYS	A	98	20.208	42.557	3.861	1.00	43.56	N
ATOM	754	CA	LYS	A	98	18.914	42.503	4.493	1.00	50.07	C
ATOM	755	C	LYS	A	98	18.988	41.436	5.594	1.00	45.12	C
ATOM	756	O	LYS	A	98	19.772	40.483	5.518	1.00	44.19	O
ATOM	757	CB	LYS	A	98	17.835	42.141	3.467	1.00	42.89	C
ATOM	758	CG	LYS	A	98	17.806	40.689	3.029	1.00	54.06	C
ATOM	759	CD	LYS	A	98	16.620	40.432	2.091	1.00	70.03	C
ATOM	760	CE	LYS	A	98	16.542	38.972	1.674	1.00	74.47	C
ATOM	761	NZ	LYS	A	98	15.366	38.722	0.799	1.00	87.06	N
ATOM	762	N	LEU	A	99	18.187	41.633	6.625	1.00	42.33	N
ATOM	763	CA	LEU	A	99	18.112	40.718	7.743	1.00	48.11	C
ATOM	764	C	LEU	A	99	17.731	39.322	7.271	1.00	51.43	C
ATOM	765	O	LEU	A	99	16.622	39.119	6.784	1.00	54.69	O
ATOM	766	CB	LEU	A	99	17.058	41.223	8.727	1.00	40.97	C
ATOM	767	CG	LEU	A	99	16.874	40.365	9.974	1.00	51.52	C
ATOM	768	CD1	LEU	A	99	18.114	40.494	10.829	1.00	49.68	C
ATOM	769	CD2	LEU	A	99	15.663	40.822	10.765	1.00	51.15	C
ATOM	770	N	MET	A	100	18.643	38.358	7.388	1.00	48.12	N
ATOM	771	CA	MET	A	100	18.321	36.984	6.995	1.00	51.56	C
ATOM	772	C	MET	A	100	19.033	35.977	7.907	1.00	51.77	C
ATOM	773	O	MET	A	100	19.991	36.322	8.621	1.00	39.76	O
ATOM	774	CB	MET	A	100	18.650	36.727	5.512	1.00	61.21	C
ATOM	775	CG	MET	A	100	20.116	36.564	5.166	1.00	69.49	C
ATOM	776	SD	MET	A	100	20.416	36.505	3.372	1.00	84.60	S
ATOM	777	CE	MET	A	100	19.818	34.884	2.949	1.00	92.44	C
ATOM	778	N	PHE	A	101	18.531	34.745	7.908	1.00	45.49	N
ATOM	779	CA	PHE	A	101	19.085	33.684	8.732	1.00	50.26	C
ATOM	780	C	PHE	A	101	20.138	32.893	7.995	1.00	43.40	C
ATOM	781	O	PHE	A	101	19.907	32.400	6.902	1.00	61.65	O
ATOM	782	CB	PHE	A	101	17.969	32.769	9.210	1.00	46.80	C
ATOM	783	CG	PHE	A	101	17.019	33.450	10.137	1.00	46.54	C
ATOM	784	CD1	PHE	A	101	15.900	34.112	9.652	1.00	52.32	C
ATOM	785	CD2	PHE	A	101	17.274	33.488	11.499	1.00	44.46	C
ATOM	786	CE1	PHE	A	101	15.054	34.822	10.516	1.00	43.20	C
ATOM	787	CE2	PHE	A	101	16.441	34.192	12.366	1.00	48.20	C
ATOM	788	CZ	PHE	A	101	15.322	34.858	11.869	1.00	48.40	C
ATOM	789	N	LYS	A	102	21.302	32.771	8.611	1.00	51.46	N
ATOM	790	CA	LYS	A	102	22.420	32.066	8.009	1.00	48.23	C
ATOM	791	C	LYS	A	102	22.516	30.619	8.468	1.00	54.86	C
ATOM	792	O	LYS	A	102	22.768	29.712	7.668	1.00	62.07	O
ATOM	793	CB	LYS	A	102	23.714	32.799	8.340	1.00	57.97	C

Figure 2 (Table 2 (page 22))

ATOM	794	CG	LYS	A	102	24.954	32.199	7.720	1.00	71.82	C
ATOM	795	CD	LYS	A	102	26.170	33.021	8.108	1.00	82.19	C
ATOM	796	CE	LYS	A	102	27.335	32.773	7.169	1.00	88.42	C
ATOM	797	NZ	LYS	A	102	28.516	33.602	7.540	1.00	98.10	N
ATOM	798	N	ASN	A	103	22.328	30.409	9.763	1.00	47.83	N
ATOM	799	CA	ASN	A	103	22.379	29.081	10.339	1.00	43.78	C
ATOM	800	C	ASN	A	103	21.419	29.084	11.525	1.00	45.04	C
ATOM	801	O	ASN	A	103	21.661	29.751	12.534	1.00	40.24	O
ATOM	802	CB	ASN	A	103	23.802	28.764	10.800	1.00	45.29	C
ATOM	803	CG	ASN	A	103	23.886	27.468	11.565	1.00	46.73	C
ATOM	804	OD1	ASN	A	103	23.582	26.402	11.037	1.00	54.61	O
ATOM	805	ND2	ASN	A	103	24.308	27.552	12.822	1.00	50.10	N
ATOM	806	N	ALA	A	104	20.312	28.369	11.379	1.00	40.89	N
ATOM	807	CA	ALA	A	104	19.304	28.264	12.422	1.00	48.41	C
ATOM	808	C	ALA	A	104	18.651	26.906	12.200	1.00	52.07	C
ATOM	809	O	ALA	A	104	17.490	26.811	11.829	1.00	51.94	O
ATOM	810	CB	ALA	A	104	18.280	29.359	12.241	1.00	53.18	C
ATOM	811	N	PRO	A	105	19.386	25.834	12.461	1.00	47.52	N
ATOM	812	CA	PRO	A	105	18.873	24.481	12.265	1.00	45.57	C
ATOM	813	C	PRO	A	105	17.700	24.096	13.112	1.00	47.49	C
ATOM	814	O	PRO	A	105	17.508	24.606	14.223	1.00	41.72	O
ATOM	815	CB	PRO	A	105	20.087	23.588	12.501	1.00	49.47	C
ATOM	816	CG	PRO	A	105	21.055	24.460	13.270	1.00	52.18	C
ATOM	817	CD	PRO	A	105	20.631	25.867	13.230	1.00	52.90	C
ATOM	818	N	THR	A	106	16.864	23.260	12.515	1.00	48.69	N
ATOM	819	CA	THR	A	106	15.717	22.758	13.215	1.00	52.32	C
ATOM	820	C	THR	A	106	15.529	21.322	12.759	1.00	58.90	C
ATOM	821	O	THR	A	106	15.672	20.999	11.581	1.00	55.09	O
ATOM	822	CB	THR	A	106	14.447	23.612	12.955	1.00	53.67	C
ATOM	823	OG1	THR	A	106	13.355	23.053	13.698	1.00	54.59	O
ATOM	824	CG2	THR	A	106	14.097	23.641	11.468	1.00	58.16	C
ATOM	825	N	PRO	A	107	15.275	20.424	13.714	1.00	52.16	N
ATOM	826	CA	PRO	A	107	15.184	20.737	15.138	1.00	43.22	C
ATOM	827	C	PRO	A	107	16.585	20.810	15.732	1.00	47.05	C
ATOM	828	O	PRO	A	107	17.578	20.532	15.064	1.00	45.59	O
ATOM	829	CB	PRO	A	107	14.426	19.539	15.688	1.00	49.39	C
ATOM	830	CG	PRO	A	107	15.052	18.411	14.902	1.00	55.45	C
ATOM	831	CD	PRO	A	107	15.065	18.986	13.480	1.00	55.64	C
ATOM	832	N	GLN	A	108	16.650	21.202	16.994	1.00	40.58	N
ATOM	833	CA	GLN	A	108	17.901	21.229	17.709	1.00	46.97	C
ATOM	834	C	GLN	A	108	17.566	20.339	18.896	1.00	44.47	C
ATOM	835	O	GLN	A	108	16.492	20.467	19.489	1.00	36.69	O
ATOM	836	CB	GLN	A	108	18.271	22.657	18.084	1.00	40.68	C
ATOM	837	CG	GLN	A	108	18.770	23.436	16.846	1.00	37.05	C
ATOM	838	CD	GLN	A	108	19.203	24.847	17.171	1.00	40.43	C
ATOM	839	OE1	GLN	A	108	19.879	25.073	18.172	1.00	36.29	O
ATOM	840	NE2	GLN	A	108	18.828	25.805	16.332	1.00	37.82	N
ATOM	841	N	GLU	A	109	18.469	19.413	19.203	1.00	38.32	N
ATOM	842	CA	GLU	A	109	18.261	18.425	20.257	1.00	39.59	C
ATOM	843	C	GLU	A	109	19.216	18.551	21.424	1.00	44.20	C
ATOM	844	O	GLU	A	109	20.380	18.922	21.254	1.00	41.88	O
ATOM	845	CB	GLU	A	109	18.364	17.033	19.637	1.00	39.87	C
ATOM	846	CG	GLU	A	109	17.437	16.885	18.448	1.00	45.54	C
ATOM	847	CD	GLU	A	109	17.358	15.478	17.912	1.00	49.95	C
ATOM	848	OE1	GLU	A	109	17.335	14.518	18.713	1.00	54.48	O
ATOM	849	OE2	GLU	A	109	17.295	15.330	16.678	1.00	54.37	O

Figure 2 (Table 2 (page 23))

ATOM	850	N	PHE	A	110	18.713	18.223	22.609	1.00	36.31	N
ATOM	851	CA	PHE	A	110	19.491	18.314	23.825	1.00	37.31	C
ATOM	852	C	PHE	A	110	19.154	17.167	24.748	1.00	44.15	C
ATOM	853	O	PHE	A	110	18.071	16.596	24.694	1.00	42.74	O
ATOM	854	CB	PHE	A	110	19.202	19.643	24.531	1.00	29.73	C
ATOM	855	CG	PHE	A	110	19.299	20.831	23.612	1.00	36.45	C
ATOM	856	CD1	PHE	A	110	18.189	21.286	22.922	1.00	37.59	C
ATOM	857	CD2	PHE	A	110	20.522	21.445	23.387	1.00	35.71	C
ATOM	858	CE1	PHE	A	110	18.301	22.337	22.006	1.00	49.86	C
ATOM	859	CE2	PHE	A	110	20.649	22.489	22.476	1.00	43.61	C
ATOM	860	CZ	PHE	A	110	19.533	22.939	21.785	1.00	39.36	C
ATOM	861	N	LYS	A	111	20.108	16.819	25.592	1.00	38.44	N
ATOM	862	CA	LYS	A	111	19.909	15.745	26.533	1.00	39.53	C
ATOM	863	C	LYS	A	111	19.327	16.395	27.769	1.00	33.66	C
ATOM	864	O	LYS	A	111	19.832	17.419	28.238	1.00	37.40	O
ATOM	865	CB	LYS	A	111	21.254	15.075	26.845	1.00	35.52	C
ATOM	866	CG	LYS	A	111	21.185	13.974	27.890	1.00	45.41	C
ATOM	867	CD	LYS	A	111	22.548	13.272	28.006	1.00	51.44	C
ATOM	868	CE	LYS	A	111	22.515	12.114	29.000	1.00	58.54	C
ATOM	869	NZ	LYS	A	111	23.657	11.172	28.765	1.00	62.26	N
ATOM	870	N	GLU	A	112	18.255	15.810	28.287	1.00	39.60	N
ATOM	871	CA	GLU	A	112	17.614	16.339	29.478	1.00	42.51	C
ATOM	872	C	GLU	A	112	18.627	16.706	30.569	1.00	37.78	C
ATOM	873	O	GLU	A	112	19.554	15.950	30.846	1.00	41.69	O
ATOM	874	CB	GLU	A	112	16.621	15.312	30.034	1.00	42.05	C
ATOM	875	CG	GLU	A	112	15.743	15.888	31.120	1.00	48.02	C
ATOM	876	CD	GLU	A	112	14.735	14.886	31.675	1.00	67.88	C
ATOM	877	OE1	GLU	A	112	13.582	15.304	31.937	1.00	64.90	O
ATOM	878	OE2	GLU	A	112	15.093	13.700	31.865	1.00	70.27	O
ATOM	879	N	GLY	A	113	18.448	17.875	31.175	1.00	41.71	N
ATOM	880	CA	GLY	A	113	19.350	18.298	32.228	1.00	43.96	C
ATOM	881	C	GLY	A	113	20.555	19.128	31.824	1.00	46.88	C
ATOM	882	O	GLY	A	113	21.087	19.877	32.652	1.00	44.90	O
ATOM	883	N	GLU	A	114	21.017	19.021	30.584	1.00	41.27	N
ATOM	884	CA	GLU	A	114	22.181	19.830	30.227	1.00	49.33	C
ATOM	885	C	GLU	A	114	21.739	21.260	29.927	1.00	46.85	C
ATOM	886	O	GLU	A	114	20.539	21.551	29.864	1.00	45.47	O
ATOM	887	CB	GLU	A	114	22.957	19.199	29.052	1.00	46.70	C
ATOM	888	CG	GLU	A	114	22.319	19.293	27.682	1.00	49.46	C
ATOM	889	CD	GLU	A	114	23.076	18.490	26.613	1.00	56.05	C
ATOM	890	OE1	GLU	A	114	24.174	17.946	26.894	1.00	59.22	O
ATOM	891	OE2	GLU	A	114	22.565	18.407	25.482	1.00	51.60	O
ATOM	892	N	ASP	A	115	22.689	22.181	29.822	1.00	42.06	N
ATOM	893	CA	ASP	A	115	22.323	23.554	29.512	1.00	46.33	C
ATOM	894	C	ASP	A	115	22.184	23.568	28.018	1.00	46.24	C
ATOM	895	O	ASP	A	115	23.107	23.195	27.299	1.00	51.16	O
ATOM	896	CB	ASP	A	115	23.394	24.525	29.976	1.00	52.16	C
ATOM	897	CG	ASP	A	115	23.530	24.535	31.475	1.00	58.98	C
ATOM	898	OD1	ASP	A	115	22.515	24.291	32.169	1.00	56.34	O
ATOM	899	OD2	ASP	A	115	24.647	24.785	31.959	1.00	74.61	O
ATOM	900	N	ALA	A	116	21.009	23.943	27.536	1.00	40.21	N
ATOM	901	CA	ALA	A	116	20.812	23.937	26.105	1.00	41.98	C
ATOM	902	C	ALA	A	116	21.024	25.315	25.524	1.00	39.57	C
ATOM	903	O	ALA	A	116	20.591	26.311	26.093	1.00	41.84	O
ATOM	904	CB	ALA	A	116	19.406	23.428	25.761	1.00	37.59	C
ATOM	905	N	VAL	A	117	21.711	25.374	24.396	1.00	35.34	N



Figure 2 (Table 2 (page 24))

ATOM	906	CA	VAL	A	117	21.907	26.651	23.736	1.00	34.85	C
ATOM	907	C	VAL	A	117	21.305	26.459	22.356	1.00	34.14	C
ATOM	908	O	VAL	A	117	21.751	25.608	21.603	1.00	35.50	O
ATOM	909	CB	VAL	A	117	23.391	26.997	23.612	1.00	40.36	C
ATOM	910	CG1	VAL	A	117	23.573	28.240	22.764	1.00	35.45	C
ATOM	911	CG2	VAL	A	117	23.957	27.265	24.994	1.00	46.40	C
ATOM	912	N	ILE	A	118	20.276	27.244	22.046	1.00	35.04	N
ATOM	913	CA	ILE	A	118	19.593	27.169	20.757	1.00	34.21	C
ATOM	914	C	ILE	A	118	20.257	28.172	19.836	1.00	25.24	C
ATOM	915	O	ILE	A	118	20.252	29.371	20.095	1.00	32.78	O
ATOM	916	CB	ILE	A	118	18.106	27.535	20.901	1.00	34.79	C
ATOM	917	CG1	ILE	A	118	17.471	26.651	21.978	1.00	43.37	C
ATOM	918	CG2	ILE	A	118	17.384	27.289	19.578	1.00	35.72	C
ATOM	919	CD1	ILE	A	118	16.071	27.043	22.340	1.00	58.55	C
ATOM	920	N	VAL	A	119	20.829	27.649	18.771	1.00	31.01	N
ATOM	921	CA	VAL	A	119	21.593	28.441	17.830	1.00	37.30	C
ATOM	922	C	VAL	A	119	20.771	29.119	16.753	1.00	37.56	C
ATOM	923	O	VAL	A	119	19.983	28.491	16.065	1.00	40.50	O
ATOM	924	CB	VAL	A	119	22.670	27.549	17.175	1.00	35.82	C
ATOM	925	CG1	VAL	A	119	23.467	28.340	16.136	1.00	34.06	C
ATOM	926	CG2	VAL	A	119	23.582	27.004	18.258	1.00	34.59	C
ATOM	927	N	CYS	A	120	20.980	30.414	16.620	1.00	36.81	N
ATOM	928	CA	CYS	A	120	20.286	31.194	15.610	1.00	32.12	C
ATOM	929	C	CYS	A	120	21.262	32.279	15.148	1.00	33.42	C
ATOM	930	O	CYS	A	120	21.534	33.244	15.873	1.00	34.81	O
ATOM	931	CB	CYS	A	120	19.027	31.819	16.211	1.00	41.13	C
ATOM	932	SG	CYS	A	120	17.972	32.754	15.028	1.00	50.41	S
ATOM	933	N	ASP	A	121	21.821	32.082	13.959	1.00	36.26	N
ATOM	934	CA	ASP	A	121	22.778	33.020	13.370	1.00	38.88	C
ATOM	935	C	ASP	A	121	22.109	33.906	12.333	1.00	36.35	C
ATOM	936	O	ASP	A	121	21.607	33.429	11.326	1.00	41.43	O
ATOM	937	CB	ASP	A	121	23.934	32.251	12.720	1.00	41.76	C
ATOM	938	CG	ASP	A	121	24.766	31.509	13.744	1.00	40.59	C
ATOM	939	OD1	ASP	A	121	25.129	32.153	14.749	1.00	47.54	O
ATOM	940	OD2	ASP	A	121	25.047	30.306	13.560	1.00	45.40	O
ATOM	941	N	VAL	A	122	22.099	35.202	12.584	1.00	41.75	N
ATOM	942	CA	VAL	A	122	21.495	36.119	11.636	1.00	52.79	C
ATOM	943	C	VAL	A	122	22.563	36.999	11.025	1.00	52.22	C
ATOM	944	O	VAL	A	122	23.670	37.115	11.550	1.00	45.91	O
ATOM	945	CB	VAL	A	122	20.458	37.052	12.302	1.00	53.37	C
ATOM	946	CG1	VAL	A	122	19.391	36.242	12.998	1.00	50.48	C
ATOM	947	CG2	VAL	A	122	21.153	37.986	13.275	1.00	58.84	C
ATOM	948	N	VAL	A	123	22.215	37.609	9.901	1.00	47.92	N
ATOM	949	CA	VAL	A	123	23.104	38.525	9.211	1.00	44.45	C
ATOM	950	C	VAL	A	123	22.279	39.739	8.809	1.00	53.24	C
ATOM	951	O	VAL	A	123	21.097	39.610	8.449	1.00	44.25	O
ATOM	952	CB	VAL	A	123	23.713	37.910	7.941	1.00	53.12	C
ATOM	953	CG1	VAL	A	123	24.633	36.758	8.307	1.00	58.99	C
ATOM	954	CG2	VAL	A	123	22.610	37.442	7.012	1.00	54.51	C
ATOM	955	N	SER	A	124	22.911	40.906	8.893	1.00	38.99	N
ATOM	956	CA	SER	A	124	22.304	42.181	8.537	1.00	42.72	C
ATOM	957	C	SER	A	124	23.383	43.252	8.618	1.00	46.36	C
ATOM	958	O	SER	A	124	24.311	43.139	9.420	1.00	48.23	O
ATOM	959	CB	SER	A	124	21.169	42.533	9.496	1.00	45.26	C
ATOM	960	OG	SER	A	124	21.642	42.618	10.828	1.00	50.88	O
ATOM	961	N	SER	A	125	23.257	44.283	7.787	1.00	48.24	N

Figure 2 (Table 2 (page 25))

ATOM	962	CA	SER	A	125	24.221	45.387	7.755	1.00	54.08	C
ATOM	963	C	SER	A	125	24.173	46.098	9.081	1.00	53.53	C
ATOM	964	O	SER	A	125	25.201	46.357	9.694	1.00	54.81	O
ATOM	965	CB	SER	A	125	23.874	46.373	6.641	1.00	45.61	C
ATOM	966	OG	SER	A	125	23.901	45.724	5.391	1.00	46.33	O
ATOM	967	N	LEU	A	126	22.961	46.408	9.519	1.00	51.93	N
ATOM	968	CA	LEU	A	126	22.756	47.077	10.795	1.00	60.20	C
ATOM	969	C	LEU	A	126	22.575	46.030	11.889	1.00	63.51	C
ATOM	970	O	LEU	A	126	22.012	44.961	11.657	1.00	63.28	O
ATOM	971	CB	LEU	A	126	21.521	47.987	10.726	1.00	67.31	C
ATOM	972	CG	LEU	A	126	21.606	49.171	9.746	1.00	75.52	C
ATOM	973	CD1	LEU	A	126	20.323	49.998	9.750	1.00	66.85	C
ATOM	974	CD2	LEU	A	126	22.791	50.045	10.141	1.00	72.14	C
ATOM	975	N	PRO	A	127	23.071	46.308	13.096	1.00	69.25	N
ATOM	976	CA	PRO	A	127	22.925	45.331	14.185	1.00	64.19	C
ATOM	977	C	PRO	A	127	21.463	45.007	14.524	1.00	57.99	C
ATOM	978	O	PRO	A	127	20.655	45.913	14.728	1.00	62.20	O
ATOM	979	CB	PRO	A	127	23.701	45.950	15.354	1.00	64.92	C
ATOM	980	CG	PRO	A	127	23.957	47.367	14.952	1.00	66.17	C
ATOM	981	CD	PRO	A	127	23.849	47.492	13.478	1.00	65.55	C
ATOM	982	N	PRO	A	128	21.126	43.698	14.610	1.00	61.71	N
ATOM	983	CA	PRO	A	128	19.782	43.195	14.906	1.00	61.85	C
ATOM	984	C	PRO	A	128	19.470	43.143	16.362	1.00	62.11	C
ATOM	985	O	PRO	A	128	20.351	42.980	17.192	1.00	64.26	O
ATOM	986	CB	PRO	A	128	19.805	41.776	14.340	1.00	58.63	C
ATOM	987	CG	PRO	A	128	21.070	41.714	13.493	1.00	66.61	C
ATOM	988	CD	PRO	A	128	22.009	42.561	14.287	1.00	51.57	C
ATOM	989	N	THR	A	129	18.196	43.270	16.669	1.00	56.05	N
ATOM	990	CA	THR	A	129	17.759	43.128	18.039	1.00	50.88	C
ATOM	991	C	THR	A	129	17.038	41.791	17.944	1.00	47.70	C
ATOM	992	O	THR	A	129	16.192	41.597	17.072	1.00	52.86	O
ATOM	993	CB	THR	A	129	16.801	44.243	18.457	1.00	59.29	C
ATOM	994	OG1	THR	A	129	17.564	45.360	18.933	1.00	64.98	O
ATOM	995	CG2	THR	A	129	15.885	43.769	19.562	1.00	68.98	C
ATOM	996	N	ILE	A	130	17.377	40.868	18.827	1.00	47.42	N
ATOM	997	CA	ILE	A	130	16.793	39.543	18.779	1.00	49.45	C
ATOM	998	C	ILE	A	130	15.829	39.251	19.914	1.00	48.06	C
ATOM	999	O	ILE	A	130	16.119	39.539	21.074	1.00	49.48	O
ATOM	1000	CB	ILE	A	130	17.907	38.480	18.805	1.00	52.16	C
ATOM	1001	CG1	ILE	A	130	18.711	38.558	17.510	1.00	55.93	C
ATOM	1002	CG2	ILE	A	130	17.317	37.091	19.030	1.00	46.63	C
ATOM	1003	CD1	ILE	A	130	17.934	38.126	16.313	1.00	58.84	C
ATOM	1004	N	ILE	A	131	14.681	38.675	19.568	1.00	45.61	N
ATOM	1005	CA	ILE	A	131	13.707	38.318	20.588	1.00	50.29	C
ATOM	1006	C	ILE	A	131	13.352	36.859	20.427	1.00	33.83	C
ATOM	1007	O	ILE	A	131	12.993	36.426	19.330	1.00	50.28	O
ATOM	1008	CB	ILE	A	131	12.374	39.104	20.474	1.00	55.23	C
ATOM	1009	CG1	ILE	A	131	12.620	40.610	20.479	1.00	61.34	C
ATOM	1010	CG2	ILE	A	131	11.470	38.737	21.647	1.00	58.84	C
ATOM	1011	CD1	ILE	A	131	12.630	41.236	19.085	1.00	60.34	C
ATOM	1012	N	TRP	A	132	13.437	36.108	21.520	1.00	38.49	N
ATOM	1013	CA	TRP	A	132	13.095	34.692	21.510	1.00	46.49	C
ATOM	1014	C	TRP	A	132	11.668	34.498	22.042	1.00	48.20	C
ATOM	1015	O	TRP	A	132	11.343	34.949	23.133	1.00	45.37	O
ATOM	1016	CB	TRP	A	132	14.085	33.898	22.372	1.00	39.62	C
ATOM	1017	CG	TRP	A	132	15.384	33.632	21.653	1.00	39.42	C

Figure 2 (Table 2 (page 26))

ATOM	1018	CD1	TRP	A	132	16.536	34.369	21.728	1.00	36.55	C
ATOM	1019	CD2	TRP	A	132	15.645	32.570	20.726	1.00	29.03	C
ATOM	1020	NE1	TRP	A	132	17.502	33.826	20.901	1.00	34.64	N
ATOM	1021	CE2	TRP	A	132	16.985	32.725	20.278	1.00	35.20	C
ATOM	1022	CE3	TRP	A	132	14.883	31.502	20.229	1.00	33.72	C
ATOM	1023	CZ2	TRP	A	132	17.572	31.848	19.364	1.00	32.11	C
ATOM	1024	CZ3	TRP	A	132	15.470	30.632	19.318	1.00	35.81	C
ATOM	1025	CH2	TRP	A	132	16.809	30.814	18.893	1.00	33.40	C
ATOM	1026	N	LYS	A	133	10.838	33.809	21.266	1.00	51.27	N
ATOM	1027	CA	LYS	A	133	9.451	33.579	21.645	1.00	57.47	C
ATOM	1028	C	LYS	A	133	9.043	32.124	21.741	1.00	59.45	C
ATOM	1029	O	LYS	A	133	9.408	31.298	20.903	1.00	53.79	O
ATOM	1030	CB	LYS	A	133	8.518	34.267	20.650	1.00	55.78	C
ATOM	1031	CG	LYS	A	133	8.672	35.771	20.593	1.00	66.61	C
ATOM	1032	CD	LYS	A	133	7.816	36.347	19.483	1.00	76.13	C
ATOM	1033	CE	LYS	A	133	7.989	37.857	19.385	1.00	82.76	C
ATOM	1034	NZ	LYS	A	133	7.076	38.469	18.372	1.00	81.20	N
ATOM	1035	N	HIS	A	134	8.274	31.824	22.781	1.00	63.05	N
ATOM	1036	CA	HIS	A	134	7.757	30.481	22.990	1.00	66.48	C
ATOM	1037	C	HIS	A	134	6.265	30.612	23.220	1.00	77.89	C
ATOM	1038	O	HIS	A	134	5.832	31.403	24.067	1.00	63.07	O
ATOM	1039	CB	HIS	A	134	8.370	29.816	24.221	1.00	70.22	C
ATOM	1040	CG	HIS	A	134	8.006	28.368	24.367	1.00	72.09	C
ATOM	1041	ND1	HIS	A	134	8.057	27.704	25.574	1.00	72.16	N
ATOM	1042	CD2	HIS	A	134	7.622	27.448	23.447	1.00	73.41	C
ATOM	1043	CE1	HIS	A	134	7.723	26.440	25.392	1.00	77.82	C
ATOM	1044	NE2	HIS	A	134	7.454	26.257	24.112	1.00	78.13	N
ATOM	1045	N	LYS	A	135	5.488	29.843	22.461	1.00	81.08	N
ATOM	1046	CA	LYS	A	135	4.034	29.850	22.574	1.00	91.79	C
ATOM	1047	C	LYS	A	135	3.435	31.264	22.532	1.00	92.61	C
ATOM	1048	O	LYS	A	135	2.397	31.511	23.139	1.00	95.56	O
ATOM	1049	CB	LYS	A	135	3.608	29.135	23.870	1.00	90.50	C
ATOM	1050	CG	LYS	A	135	3.832	29.955	25.143	1.00	96.62	C
ATOM	1051	CD	LYS	A	135	3.541	29.173	26.414	1.00	94.31	C
ATOM	1052	CE	LYS	A	135	3.714	30.058	27.643	1.00	94.84	C
ATOM	1053	NZ	LYS	A	135	3.553	29.294	28.915	1.00	95.67	N
ATOM	1054	N	GLY	A	136	4.082	32.194	21.828	1.00	91.50	N
ATOM	1055	CA	GLY	A	136	3.553	33.551	21.741	1.00	88.54	C
ATOM	1056	C	GLY	A	136	4.256	34.597	22.589	1.00	85.72	C
ATOM	1057	O	GLY	A	136	4.366	35.754	22.187	1.00	89.77	O
ATOM	1058	N	ARG	A	137	4.734	34.184	23.757	1.00	82.42	N
ATOM	1059	CA	ARG	A	137	5.426	35.064	24.698	1.00	83.81	C
ATOM	1060	C	ARG	A	137	6.867	35.398	24.329	1.00	80.74	C
ATOM	1061	O	ARG	A	137	7.372	35.029	23.272	1.00	83.63	O
ATOM	1062	CB	ARG	A	137	5.448	34.419	26.090	1.00	90.23	C
ATOM	1063	CG	ARG	A	137	4.111	34.360	26.790	1.00	99.62	C
ATOM	1064	CD	ARG	A	137	3.856	35.652	27.530	1.00	105.25	C
ATOM	1065	NE	ARG	A	137	2.445	36.009	27.526	1.00	113.79	N
ATOM	1066	CZ	ARG	A	137	1.973	37.181	27.937	1.00	114.75	C
ATOM	1067	NH1	ARG	A	137	2.805	38.109	28.390	1.00	116.01	N
ATOM	1068	NH2	ARG	A	137	0.672	37.432	27.883	1.00	117.60	N
ATOM	1069	N	ASP	A	138	7.510	36.116	25.241	1.00	76.46	N
ATOM	1070	CA	ASP	A	138	8.907	36.497	25.132	1.00	75.03	C
ATOM	1071	C	ASP	A	138	9.464	35.773	26.328	1.00	76.03	C
ATOM	1072	O	ASP	A	138	9.139	36.102	27.476	1.00	73.85	O
ATOM	1073	CB	ASP	A	138	9.107	38.000	25.318	1.00	77.22	C

Figure 2 (Table 2 (page 27))

ATOM	1074	CG	ASP	A	138	10.578	38.403	25.275	1.00	77.41	C
ATOM	1075	OD1	ASP	A	138	11.410	37.736	25.931	1.00	76.27	O
ATOM	1076	OD2	ASP	A	138	10.906	39.394	24.590	1.00	67.17	O
ATOM	1077	N	VAL	A	139	10.292	34.776	26.069	1.00	63.30	N
ATOM	1078	CA	VAL	A	139	10.838	33.992	27.152	1.00	58.22	C
ATOM	1079	C	VAL	A	139	11.541	34.814	28.224	1.00	60.55	C
ATOM	1080	O	VAL	A	139	11.799	34.320	29.321	1.00	71.06	O
ATOM	1081	CB	VAL	A	139	11.785	32.935	26.595	1.00	62.13	C
ATOM	1082	CG1	VAL	A	139	11.091	32.195	25.469	1.00	55.43	C
ATOM	1083	CG2	VAL	A	139	13.068	33.588	26.091	1.00	47.09	C
ATOM	1084	N	ILE	A	140	11.841	36.070	27.918	1.00	66.18	N
ATOM	1085	CA	ILE	A	140	12.519	36.924	28.878	1.00	73.19	C
ATOM	1086	C	ILE	A	140	11.594	37.514	29.925	1.00	77.32	C
ATOM	1087	O	ILE	A	140	11.822	37.370	31.123	1.00	79.51	O
ATOM	1088	CB	ILE	A	140	13.229	38.098	28.183	1.00	75.30	C
ATOM	1089	CG1	ILE	A	140	14.357	37.569	27.300	1.00	79.57	C
ATOM	1090	CG2	ILE	A	140	13.789	39.062	29.227	1.00	84.41	C
ATOM	1091	CD1	ILE	A	140	15.381	36.752	28.065	1.00	75.80	C
ATOM	1092	N	LEU	A	141	10.553	38.194	29.468	1.00	85.78	N
ATOM	1093	CA	LEU	A	141	9.632	38.838	30.384	1.00	97.07	C
ATOM	1094	C	LEU	A	141	8.966	37.937	31.409	1.00	101.56	C
ATOM	1095	O	LEU	A	141	8.177	38.408	32.225	1.00	107.39	O
ATOM	1096	CB	LEU	A	141	8.571	39.615	29.608	1.00	101.80	C
ATOM	1097	CG	LEU	A	141	9.106	40.905	28.991	1.00	106.45	C
ATOM	1098	CD1	LEU	A	141	7.949	41.736	28.461	1.00	108.62	C
ATOM	1099	CD2	LEU	A	141	9.882	41.699	30.046	1.00	104.45	C
ATOM	1100	N	LYS	A	142	9.276	36.650	31.384	1.00	101.47	N
ATOM	1101	CA	LYS	A	142	8.689	35.751	32.362	1.00	101.64	C
ATOM	1102	C	LYS	A	142	9.660	35.560	33.527	1.00	101.85	C
ATOM	1103	O	LYS	A	142	9.262	35.339	34.675	1.00	105.32	O
ATOM	1104	CB	LYS	A	142	8.346	34.404	31.702	1.00	100.75	C
ATOM	1105	CG	LYS	A	142	9.525	33.643	31.098	1.00	98.61	C
ATOM	1106	CD	LYS	A	142	8.997	32.520	30.208	1.00	93.54	C
ATOM	1107	CE	LYS	A	142	10.082	31.550	29.747	1.00	96.37	C
ATOM	1108	NZ	LYS	A	142	9.503	30.522	28.822	1.00	91.06	N
ATOM	1109	N	LYS	A	143	10.940	35.703	33.223	1.00	102.59	N
ATOM	1110	CA	LYS	A	143	11.992	35.519	34.206	1.00	104.90	C
ATOM	1111	C	LYS	A	143	11.852	34.206	34.942	1.00	100.79	C
ATOM	1112	O	LYS	A	143	11.372	34.122	36.080	1.00	100.29	O
ATOM	1113	CB	LYS	A	143	12.059	36.672	35.207	1.00	107.17	C
ATOM	1114	CG	LYS	A	143	13.224	36.510	36.183	1.00	113.10	C
ATOM	1115	CD	LYS	A	143	14.559	36.248	35.522	1.00	116.78	C
ATOM	1116	CE	LYS	A	143	15.786	36.228	36.466	1.00	123.03	C
ATOM	1117	NZ	LYS	A	143	17.123	36.187	35.780	1.00	119.60	N
ATOM	1118	N	ASP	A	144	12.237	33.182	34.199	1.00	94.81	N
ATOM	1119	CA	ASP	A	144	12.319	31.828	34.669	1.00	85.45	C
ATOM	1120	C	ASP	A	144	13.827	31.840	34.531	1.00	79.96	C
ATOM	1121	O	ASP	A	144	14.365	31.687	33.436	1.00	88.63	O
ATOM	1122	CB	ASP	A	144	11.718	30.833	33.677	1.00	85.69	C
ATOM	1123	CG	ASP	A	144	11.884	29.398	34.137	1.00	89.87	C
ATOM	1124	OD1	ASP	A	144	12.989	29.060	34.609	1.00	90.66	O
ATOM	1125	OD2	ASP	A	144	10.913	28.608	34.041	1.00	101.36	O
ATOM	1126	N	VAL	A	145	14.490	32.118	35.642	1.00	68.69	N
ATOM	1127	CA	VAL	A	145	15.946	32.226	35.721	1.00	67.87	C
ATOM	1128	C	VAL	A	145	16.758	31.316	34.795	1.00	55.99	C
ATOM	1129	O	VAL	A	145	17.915	31.598	34.490	1.00	61.04	O

Figure 2 (Table 2 (page 28))

ATOM	1130	CB	VAL	A	145	16.415	31.974	37.167	1.00	76.83	C
ATOM	1131	CG1	VAL	A	145	15.901	33.082	38.076	1.00	76.29	C
ATOM	1132	CG2	VAL	A	145	15.902	30.617	37.655	1.00	77.74	C
ATOM	1133	N	ARG	A	146	16.148	30.227	34.349	1.00	52.68	N
ATOM	1134	CA	ARG	A	146	16.839	29.283	33.493	1.00	56.85	C
ATOM	1135	C	ARG	A	146	16.984	29.771	32.055	1.00	48.40	C
ATOM	1136	O	ARG	A	146	17.808	29.258	31.311	1.00	46.31	O
ATOM	1137	CB	ARG	A	146	16.121	27.925	33.538	1.00	44.42	C
ATOM	1138	CG	ARG	A	146	16.235	27.242	34.901	1.00	53.27	C
ATOM	1139	CD	ARG	A	146	15.613	25.846	34.911	1.00	47.00	C
ATOM	1140	NE	ARG	A	146	14.253	25.864	34.388	1.00	43.57	N
ATOM	1141	CZ	ARG	A	146	13.898	25.279	33.253	1.00	53.19	C
ATOM	1142	NH1	ARG	A	146	14.810	24.627	32.533	1.00	46.06	N
ATOM	1143	NH2	ARG	A	146	12.646	25.359	32.825	1.00	49.59	N
ATOM	1144	N	PHE	A	147	16.190	30.766	31.680	1.00	49.96	N
ATOM	1145	CA	PHE	A	147	16.233	31.297	30.330	1.00	55.08	C
ATOM	1146	C	PHE	A	147	17.068	32.568	30.213	1.00	55.40	C
ATOM	1147	O	PHE	A	147	16.837	33.551	30.916	1.00	58.84	O
ATOM	1148	CB	PHE	A	147	14.815	31.536	29.828	1.00	47.49	C
ATOM	1149	CG	PHE	A	147	14.003	30.271	29.679	1.00	55.00	C
ATOM	1150	CD1	PHE	A	147	13.520	29.598	30.796	1.00	50.35	C
ATOM	1151	CD2	PHE	A	147	13.730	29.747	28.416	1.00	49.95	C
ATOM	1152	CE1	PHE	A	147	12.773	28.416	30.654	1.00	61.13	C
ATOM	1153	CE2	PHE	A	147	12.986	28.571	28.265	1.00	53.83	C
ATOM	1154	CZ	PHE	A	147	12.508	27.905	29.386	1.00	56.75	C
ATOM	1155	N	ILE	A	148	18.038	32.536	29.307	1.00	50.18	N
ATOM	1156	CA	ILE	A	148	18.940	33.661	29.097	1.00	53.42	C
ATOM	1157	C	ILE	A	148	19.348	33.856	27.636	1.00	45.25	C
ATOM	1158	O	ILE	A	148	19.659	32.899	26.944	1.00	44.46	O
ATOM	1159	CB	ILE	A	148	20.233	33.463	29.908	1.00	55.88	C
ATOM	1160	CG1	ILE	A	148	19.907	33.427	31.399	1.00	65.94	C
ATOM	1161	CG2	ILE	A	148	21.231	34.573	29.597	1.00	61.53	C
ATOM	1162	CD1	ILE	A	148	21.093	33.081	32.279	1.00	69.07	C
ATOM	1163	N	VAL	A	149	19.337	35.099	27.172	1.00	37.73	N
ATOM	1164	CA	VAL	A	149	19.764	35.381	25.817	1.00	42.64	C
ATOM	1165	C	VAL	A	149	21.236	35.794	25.962	1.00	46.84	C
ATOM	1166	O	VAL	A	149	21.552	36.756	26.655	1.00	47.29	O
ATOM	1167	CB	VAL	A	149	18.929	36.512	25.185	1.00	42.61	C
ATOM	1168	CG1	VAL	A	149	19.472	36.844	23.791	1.00	44.21	C
ATOM	1169	CG2	VAL	A	149	17.444	36.067	25.064	1.00	43.57	C
ATOM	1170	N	LEU	A	150	22.127	35.036	25.328	1.00	40.34	N
ATOM	1171	CA	LEU	A	150	23.568	35.289	25.400	1.00	42.16	C
ATOM	1172	C	LEU	A	150	24.030	36.450	24.524	1.00	47.24	C
ATOM	1173	O	LEU	A	150	23.262	36.965	23.723	1.00	39.70	O
ATOM	1174	CB	LEU	A	150	24.305	34.019	25.001	1.00	36.82	C
ATOM	1175	CG	LEU	A	150	23.885	32.825	25.860	1.00	50.79	C
ATOM	1176	CD1	LEU	A	150	24.330	31.505	25.225	1.00	45.07	C
ATOM	1177	CD2	LEU	A	150	24.473	32.999	27.252	1.00	55.15	C
ATOM	1178	N	SER	A	151	25.295	36.849	24.666	1.00	50.63	N
ATOM	1179	CA	SER	A	151	25.849	37.953	23.880	1.00	44.74	C
ATOM	1180	C	SER	A	151	25.770	37.710	22.365	1.00	37.06	C
ATOM	1181	O	SER	A	151	25.651	38.663	21.587	1.00	49.84	O
ATOM	1182	CB	SER	A	151	27.320	38.200	24.273	1.00	45.09	C
ATOM	1183	OG	SER	A	151	28.150	37.144	23.792	1.00	45.86	O
ATOM	1184	N	ASN	A	152	25.866	36.455	21.937	1.00	38.65	N
ATOM	1185	CA	ASN	A	152	25.784	36.140	20.506	1.00	40.49	C

Figure 2 (Table 2 (page 29))

ATOM	1186	C	ASN A 152	24.321	35.998	20.073	1.00	40.22	C
ATOM	1187	O	ASN A 152	24.036	35.583	18.936	1.00	34.75	O
ATOM	1188	CB	ASN A 152	26.476	34.821	20.207	1.00	39.82	C
ATOM	1189	CG	ASN A 152	26.097	33.752	21.199	1.00	54.90	C
ATOM	1190	OD1	ASN A 152	24.972	33.739	21.694	1.00	45.34	O
ATOM	1191	ND2	ASN A 152	27.029	32.850	21.504	1.00	46.13	N
ATOM	1192	N	ASN A 153	23.410	36.309	20.990	1.00	38.94	N
ATOM	1193	CA	ASN A 153	21.969	36.213	20.740	1.00	45.44	C
ATOM	1194	C	ASN A 153	21.352	34.827	20.723	1.00	42.99	C
ATOM	1195	O	ASN A 153	20.171	34.674	20.414	1.00	38.19	O
ATOM	1196	CB	ASN A 153	21.589	36.964	19.469	1.00	42.88	C
ATOM	1197	CG	ASN A 153	21.665	38.468	19.660	1.00	49.74	C
ATOM	1198	OD1	ASN A 153	21.300	38.990	20.720	1.00	57.35	O
ATOM	1199	ND2	ASN A 153	22.130	39.171	18.645	1.00	53.13	N
ATOM	1200	N	TYR A 154	22.121	33.810	21.080	1.00	31.78	N
ATOM	1201	CA	TYR A 154	21.563	32.463	21.151	1.00	37.05	C
ATOM	1202	C	TYR A 154	20.707	32.352	22.418	1.00	36.11	C
ATOM	1203	O	TYR A 154	20.918	33.107	23.357	1.00	35.56	O
ATOM	1204	CB	TYR A 154	22.675	31.425	21.247	1.00	35.50	C
ATOM	1205	CG	TYR A 154	23.535	31.329	20.021	1.00	40.10	C
ATOM	1206	CD1	TYR A 154	24.703	30.565	20.037	1.00	33.69	C
ATOM	1207	CD2	TYR A 154	23.179	31.990	18.837	1.00	35.06	C
ATOM	1208	CE1	TYR A 154	25.505	30.457	18.899	1.00	38.35	C
ATOM	1209	CE2	TYR A 154	23.979	31.892	17.676	1.00	34.58	C
ATOM	1210	CZ	TYR A 154	25.143	31.119	17.726	1.00	46.30	C
ATOM	1211	OH	TYR A 154	25.954	31.005	16.618	1.00	43.90	O
ATOM	1212	N	LEU A 155	19.757	31.415	22.450	1.00	37.10	N
ATOM	1213	CA	LEU A 155	18.936	31.237	23.650	1.00	33.06	C
ATOM	1214	C	LEU A 155	19.514	30.121	24.496	1.00	25.37	C
ATOM	1215	O	LEU A 155	19.688	28.989	24.037	1.00	33.57	O
ATOM	1216	CB	LEU A 155	17.482	30.866	23.303	1.00	33.13	C
ATOM	1217	CG	LEU A 155	16.635	30.561	24.545	1.00	39.86	C
ATOM	1218	CD1	LEU A 155	16.673	31.752	25.480	1.00	39.38	C
ATOM	1219	CD2	LEU A 155	15.185	30.269	24.142	1.00	35.14	C
ATOM	1220	N	GLN A 156	19.802	30.437	25.746	1.00	34.79	N
ATOM	1221	CA	GLN A 156	20.327	29.432	26.638	1.00	30.99	C
ATOM	1222	C	GLN A 156	19.212	28.964	27.568	1.00	33.82	C
ATOM	1223	O	GLN A 156	18.545	29.792	28.205	1.00	38.51	O
ATOM	1224	CB	GLN A 156	21.454	30.010	27.507	1.00	36.98	C
ATOM	1225	CG	GLN A 156	22.028	28.974	28.478	1.00	52.10	C
ATOM	1226	CD	GLN A 156	23.034	29.556	29.461	1.00	59.17	C
ATOM	1227	OE1	GLN A 156	22.750	30.542	30.134	1.00	58.98	O
ATOM	1228	NE2	GLN A 156	24.207	28.934	29.558	1.00	56.95	N
ATOM	1229	N	ILE A 157	19.012	27.651	27.655	1.00	35.15	N
ATOM	1230	CA	ILE A 157	18.001	27.104	28.570	1.00	39.14	C
ATOM	1231	C	ILE A 157	18.737	26.177	29.530	1.00	40.54	C
ATOM	1232	O	ILE A 157	19.028	25.030	29.189	1.00	41.38	O
ATOM	1233	CB	ILE A 157	16.928	26.304	27.832	1.00	36.32	C
ATOM	1234	CG1	ILE A 157	16.195	27.208	26.843	1.00	32.60	C
ATOM	1235	CG2	ILE A 157	15.943	25.728	28.842	1.00	42.84	C
ATOM	1236	CD1	ILE A 157	15.181	26.458	25.983	1.00	40.70	C
ATOM	1237	N	ARG A 158	19.068	26.674	30.718	1.00	38.99	N
ATOM	1238	CA	ARG A 158	19.804	25.857	31.673	1.00	45.51	C
ATOM	1239	C	ARG A 158	18.982	24.711	32.273	1.00	43.75	C
ATOM	1240	O	ARG A 158	17.781	24.851	32.484	1.00	47.32	O
ATOM	1241	CB	ARG A 158	20.381	26.749	32.778	1.00	53.96	C

Figure 2 (Table 2 (page 30))

ATOM	1242	CG	ARG	A	158	21.475	27.697	32.272	1.00	70.32	C
ATOM	1243	CD	ARG	A	158	22.155	28.453	33.405	1.00	65.23	C
ATOM	1244	NE	ARG	A	158	21.287	29.449	34.012	1.00	68.48	N
ATOM	1245	CZ	ARG	A	158	21.572	30.079	35.147	1.00	75.70	C
ATOM	1246	NH1	ARG	A	158	22.704	29.808	35.792	1.00	65.00	N
ATOM	1247	NH2	ARG	A	158	20.724	30.973	35.641	1.00	71.67	N
ATOM	1248	N	GLY	A	159	19.653	23.589	32.544	1.00	47.20	N
ATOM	1249	CA	GLY	A	159	18.998	22.415	33.096	1.00	48.68	C
ATOM	1250	C	GLY	A	159	17.731	22.133	32.317	1.00	50.27	C
ATOM	1251	O	GLY	A	159	16.658	21.983	32.897	1.00	44.17	O
ATOM	1252	N	ILE	A	160	17.847	22.050	30.997	1.00	46.11	N
ATOM	1253	CA	ILE	A	160	16.664	21.831	30.189	1.00	39.12	C
ATOM	1254	C	ILE	A	160	15.872	20.590	30.606	1.00	46.02	C
ATOM	1255	O	ILE	A	160	16.434	19.514	30.840	1.00	35.03	O
ATOM	1256	CB	ILE	A	160	17.013	21.755	28.702	1.00	34.52	C
ATOM	1257	CG1	ILE	A	160	15.727	21.917	27.874	1.00	37.12	C
ATOM	1258	CG2	ILE	A	160	17.679	20.446	28.376	1.00	34.14	C
ATOM	1259	CD1	ILE	A	160	15.993	22.199	26.392	1.00	28.22	C
ATOM	1260	N	LYS	A	161	14.557	20.767	30.692	1.00	42.18	N
ATOM	1261	CA	LYS	A	161	13.631	19.710	31.089	1.00	47.02	C
ATOM	1262	C	LYS	A	161	12.855	19.202	29.899	1.00	43.66	C
ATOM	1263	O	LYS	A	161	12.686	19.908	28.899	1.00	41.53	O
ATOM	1264	CB	LYS	A	161	12.599	20.236	32.095	1.00	49.68	C
ATOM	1265	CG	LYS	A	161	13.156	20.896	33.337	1.00	55.48	C
ATOM	1266	CD	LYS	A	161	12.002	21.450	34.178	1.00	65.12	C
ATOM	1267	CE	LYS	A	161	12.488	22.175	35.421	1.00	70.60	C
ATOM	1268	NZ	LYS	A	161	11.350	22.563	36.307	1.00	76.58	N
ATOM	1269	N	LYS	A	162	12.353	17.982	30.020	1.00	44.57	N
ATOM	1270	CA	LYS	A	162	11.560	17.383	28.956	1.00	47.82	C
ATOM	1271	C	LYS	A	162	10.372	18.311	28.670	1.00	43.43	C
ATOM	1272	O	LYS	A	162	9.914	18.427	27.535	1.00	44.67	O
ATOM	1273	CB	LYS	A	162	11.084	15.987	29.391	1.00	50.56	C
ATOM	1274	CG	LYS	A	162	10.298	15.208	28.339	1.00	50.30	C
ATOM	1275	CD	LYS	A	162	11.109	14.958	27.085	1.00	52.43	C
ATOM	1276	CE	LYS	A	162	10.279	14.227	26.051	1.00	60.58	C
ATOM	1277	NZ	LYS	A	162	10.963	14.149	24.731	1.00	59.55	N
ATOM	1278	N	THR	A	163	9.897	19.010	29.691	1.00	44.12	N
ATOM	1279	CA	THR	A	163	8.764	19.904	29.487	1.00	53.06	C
ATOM	1280	C	THR	A	163	9.140	21.234	28.833	1.00	55.60	C
ATOM	1281	O	THR	A	163	8.294	22.107	28.676	1.00	50.18	O
ATOM	1282	CB	THR	A	163	8.022	20.195	30.812	1.00	53.57	C
ATOM	1283	OG1	THR	A	163	8.942	20.712	31.780	1.00	55.40	O
ATOM	1284	CG2	THR	A	163	7.372	18.914	31.349	1.00	55.53	C
ATOM	1285	N	ASP	A	164	10.407	21.397	28.465	1.00	48.62	N
ATOM	1286	CA	ASP	A	164	10.826	22.628	27.810	1.00	42.03	C
ATOM	1287	C	ASP	A	164	10.764	22.477	26.299	1.00	44.90	C
ATOM	1288	O	ASP	A	164	10.821	23.470	25.573	1.00	48.57	O
ATOM	1289	CB	ASP	A	164	12.260	23.017	28.209	1.00	38.06	C
ATOM	1290	CG	ASP	A	164	12.358	23.525	29.631	1.00	36.69	C
ATOM	1291	OD1	ASP	A	164	11.469	24.295	30.052	1.00	49.63	O
ATOM	1292	OD2	ASP	A	164	13.337	23.168	30.327	1.00	44.71	O
ATOM	1293	N	GLU	A	165	10.639	21.251	25.798	1.00	44.64	N
ATOM	1294	CA	GLU	A	165	10.602	21.116	24.353	1.00	53.09	C
ATOM	1295	C	GLU	A	165	9.396	21.821	23.739	1.00	49.63	C
ATOM	1296	O	GLU	A	165	8.465	22.215	24.440	1.00	52.65	O
ATOM	1297	CB	GLU	A	165	10.681	19.650	23.909	1.00	50.75	C

Figure 2 (Table 2 (page 31))

ATOM	1298	CG	GLU	A	165	9.828	18.702	24.683	1.00	65.76	C
ATOM	1299	CD	GLU	A	165	9.940	17.283	24.155	1.00	72.74	C
ATOM	1300	OE1	GLU	A	165	11.040	16.884	23.691	1.00	69.18	O
ATOM	1301	OE2	GLU	A	165	8.922	16.565	24.220	1.00	65.52	O
ATOM	1302	N	GLY	A	166	9.451	22.002	22.424	1.00	48.94	N
ATOM	1303	CA	GLY	A	166	8.405	22.700	21.701	1.00	55.73	C
ATOM	1304	C	GLY	A	166	9.067	23.579	20.655	1.00	47.37	C
ATOM	1305	O	GLY	A	166	10.256	23.419	20.340	1.00	47.39	O
ATOM	1306	N	THR	A	167	8.317	24.517	20.112	0.50	34.99	N
ATOM	1307	CA	THR	A	167	8.865	25.386	19.099	0.50	35.61	C
ATOM	1308	C	THR	A	167	9.253	26.706	19.720	0.50	31.90	C
ATOM	1309	O	THR	A	167	8.524	27.264	20.526	0.50	30.91	O
ATOM	1310	CB	THR	A	167	7.849	25.623	18.006	0.50	40.53	C
ATOM	1311	OG1	THR	A	167	6.633	26.081	18.602	0.50	51.84	O
ATOM	1312	CG2	THR	A	167	7.574	24.332	17.258	0.50	26.00	C
ATOM	1313	N	TYR	A	168	10.434	27.191	19.360	1.00	43.71	N
ATOM	1314	CA	TYR	A	168	10.922	28.467	19.871	1.00	42.97	C
ATOM	1315	C	TYR	A	168	11.183	29.372	18.689	1.00	38.98	C
ATOM	1316	O	TYR	A	168	11.801	28.965	17.705	1.00	43.48	O
ATOM	1317	CB	TYR	A	168	12.205	28.283	20.682	1.00	44.02	C
ATOM	1318	CG	TYR	A	168	11.968	27.702	22.047	1.00	36.86	C
ATOM	1319	CD1	TYR	A	168	11.676	26.353	22.206	1.00	38.88	C
ATOM	1320	CD2	TYR	A	168	12.000	28.512	23.179	1.00	36.72	C
ATOM	1321	CE1	TYR	A	168	11.419	25.821	23.466	1.00	41.93	C
ATOM	1322	CE2	TYR	A	168	11.739	27.997	24.440	1.00	42.88	C
ATOM	1323	CZ	TYR	A	168	11.451	26.652	24.576	1.00	43.41	C
ATOM	1324	OH	TYR	A	168	11.193	26.139	25.824	1.00	40.88	O
ATOM	1325	N	ARG	A	169	10.715	30.610	18.787	1.00	44.05	N
ATOM	1326	CA	ARG	A	169	10.871	31.533	17.681	1.00	41.18	C
ATOM	1327	C	ARG	A	169	12.013	32.526	17.868	1.00	36.73	C
ATOM	1328	O	ARG	A	169	12.102	33.216	18.877	1.00	40.52	O
ATOM	1329	CB	ARG	A	169	9.552	32.289	17.444	1.00	50.40	C
ATOM	1330	CG	ARG	A	169	9.655	33.416	16.430	1.00	60.69	C
ATOM	1331	CD	ARG	A	169	8.284	33.861	15.925	1.00	46.23	C
ATOM	1332	NE	ARG	A	169	7.716	32.865	15.022	1.00	56.58	N
ATOM	1333	CZ	ARG	A	169	6.535	32.984	14.420	1.00	71.77	C
ATOM	1334	NH1	ARG	A	169	5.785	34.064	14.621	1.00	58.65	N
ATOM	1335	NH2	ARG	A	169	6.101	32.015	13.618	1.00	59.89	N
ATOM	1336	N	CYS	A	170	12.888	32.576	16.875	1.00	42.37	N
ATOM	1337	CA	CYS	A	170	13.998	33.506	16.919	1.00	45.65	C
ATOM	1338	C	CYS	A	170	13.546	34.667	16.025	1.00	31.99	C
ATOM	1339	O	CYS	A	170	13.423	34.505	14.810	1.00	41.21	O
ATOM	1340	CB	CYS	A	170	15.253	32.840	16.357	1.00	42.01	C
ATOM	1341	SG	CYS	A	170	16.748	33.898	16.241	1.00	52.42	S
ATOM	1342	N	GLU	A	171	13.289	35.820	16.635	1.00	44.29	N
ATOM	1343	CA	GLU	A	171	12.830	36.978	15.879	1.00	49.65	C
ATOM	1344	C	GLU	A	171	13.814	38.129	15.844	1.00	40.68	C
ATOM	1345	O	GLU	A	171	14.218	38.663	16.885	1.00	45.31	O
ATOM	1346	CB	GLU	A	171	11.503	37.502	16.426	1.00	47.28	C
ATOM	1347	CG	GLU	A	171	10.905	38.616	15.560	1.00	57.47	C
ATOM	1348	CD	GLU	A	171	9.580	39.147	16.096	1.00	65.00	C
ATOM	1349	OE1	GLU	A	171	9.593	39.989	17.028	1.00	62.15	O
ATOM	1350	OE2	GLU	A	171	8.531	38.707	15.584	1.00	54.66	O
ATOM	1351	N	GLY	A	172	14.163	38.525	14.625	1.00	46.09	N
ATOM	1352	CA	GLY	A	172	15.086	39.624	14.436	1.00	49.63	C
ATOM	1353	C	GLY	A	172	14.388	40.872	13.930	1.00	46.92	C



Figure 2 (Table 2 (page 32))

ATOM	1354	O	GLY	A	172	13.557	40.812	13.014	1.00	50.71	O
ATOM	1355	N	ARG	A	173	14.753	41.998	14.535	1.00	40.06	N
ATOM	1356	CA	ARG	A	173	14.222	43.309	14.215	1.00	44.00	C
ATOM	1357	C	ARG	A	173	15.335	44.350	14.038	1.00	56.42	C
ATOM	1358	O	ARG	A	173	16.328	44.354	14.768	1.00	47.64	O
ATOM	1359	CB	ARG	A	173	13.310	43.800	15.345	1.00	42.90	C
ATOM	1360	CG	ARG	A	173	12.048	42.970	15.527	1.00	41.21	C
ATOM	1361	CD	ARG	A	173	11.096	43.649	16.488	1.00	49.33	C
ATOM	1362	NE	ARG	A	173	9.880	42.862	16.656	1.00	55.21	N
ATOM	1363	CZ	ARG	A	173	8.669	43.387	16.790	1.00	54.70	C
ATOM	1364	NH1	ARG	A	173	8.518	44.704	16.773	1.00	54.11	N
ATOM	1365	NH2	ARG	A	173	7.610	42.596	16.935	1.00	54.36	N
ATOM	1366	N	ILE	A	174	15.135	45.245	13.080	1.00	51.94	N
ATOM	1367	CA	ILE	A	174	16.068	46.331	12.821	1.00	48.52	C
ATOM	1368	C	ILE	A	174	15.228	47.591	12.902	1.00	42.65	C
ATOM	1369	O	ILE	A	174	14.485	47.901	11.973	1.00	40.81	O
ATOM	1370	CB	ILE	A	174	16.687	46.193	11.436	1.00	51.33	C
ATOM	1371	CG1	ILE	A	174	17.536	44.921	11.395	1.00	62.03	C
ATOM	1372	CG2	ILE	A	174	17.536	47.417	11.128	1.00	57.79	C
ATOM	1373	CD1	ILE	A	174	18.075	44.586	10.042	1.00	60.04	C
ATOM	1374	N	LEU	A	175	15.348	48.327	14.004	1.00	43.83	N
ATOM	1375	CA	LEU	A	175	14.514	49.513	14.203	1.00	50.67	C
ATOM	1376	C	LEU	A	175	14.502	50.558	13.102	1.00	53.85	C
ATOM	1377	O	LEU	A	175	13.435	51.017	12.694	1.00	54.58	O
ATOM	1378	CB	LEU	A	175	14.853	50.223	15.520	1.00	52.93	C
ATOM	1379	CG	LEU	A	175	14.067	51.544	15.693	1.00	69.90	C
ATOM	1380	CD1	LEU	A	175	12.539	51.287	15.592	1.00	58.23	C
ATOM	1381	CD2	LEU	A	175	14.423	52.195	17.026	1.00	61.03	C
ATOM	1382	N	ALA	A	176	15.681	50.962	12.641	1.00	49.99	N
ATOM	1383	CA	ALA	A	176	15.753	51.981	11.605	1.00	51.23	C
ATOM	1384	C	ALA	A	176	14.902	51.629	10.385	1.00	45.44	C
ATOM	1385	O	ALA	A	176	14.347	52.518	9.739	1.00	57.30	O
ATOM	1386	CB	ALA	A	176	17.211	52.214	11.193	1.00	54.86	C
ATOM	1387	N	ARG	A	177	14.776	50.341	10.074	1.00	50.42	N
ATOM	1388	CA	ARG	A	177	13.987	49.924	8.917	1.00	45.08	C
ATOM	1389	C	ARG	A	177	12.641	49.302	9.269	1.00	48.67	C
ATOM	1390	O	ARG	A	177	11.862	48.974	8.377	1.00	45.39	O
ATOM	1391	CB	ARG	A	177	14.778	48.918	8.081	1.00	57.24	C
ATOM	1392	CG	ARG	A	177	16.084	49.467	7.544	1.00	64.35	C
ATOM	1393	CD	ARG	A	177	16.813	48.460	6.666	1.00	64.31	C
ATOM	1394	NE	ARG	A	177	17.880	49.138	5.939	1.00	77.29	N
ATOM	1395	CZ	ARG	A	177	17.889	49.331	4.625	1.00	58.44	C
ATOM	1396	NH1	ARG	A	177	16.892	48.883	3.873	1.00	54.23	N
ATOM	1397	NH2	ARG	A	177	18.884	50.009	4.074	1.00	72.33	N
ATOM	1398	N	GLY	A	178	12.373	49.130	10.562	1.00	44.96	N
ATOM	1399	CA	GLY	A	178	11.122	48.508	10.972	1.00	44.41	C
ATOM	1400	C	GLY	A	178	11.050	47.122	10.354	1.00	44.68	C
ATOM	1401	O	GLY	A	178	9.976	46.574	10.092	1.00	40.98	O
ATOM	1402	N	GLU	A	179	12.227	46.544	10.146	1.00	41.13	N
ATOM	1403	CA	GLU	A	179	12.363	45.240	9.513	1.00	46.62	C
ATOM	1404	C	GLU	A	179	12.204	44.076	10.496	1.00	46.51	C
ATOM	1405	O	GLU	A	179	12.710	44.116	11.619	1.00	46.07	O
ATOM	1406	CB	GLU	A	179	13.736	45.192	8.817	1.00	47.47	C
ATOM	1407	CG	GLU	A	179	14.011	44.049	7.852	1.00	52.61	C
ATOM	1408	CD	GLU	A	179	15.396	44.199	7.186	1.00	67.97	C
ATOM	1409	OE1	GLU	A	179	16.232	44.974	7.709	1.00	52.50	O

Figure 2 (Table 2 (page 33))

ATOM	1410	OE2	GLU	A	179	15.657	43.540	6.156	1.00	61.67	O
ATOM	1411	N	ILE	A	180	11.504	43.037	10.044	1.00	46.98	N
ATOM	1412	CA	ILE	A	180	11.260	41.843	10.844	1.00	44.57	C
ATOM	1413	C	ILE	A	180	11.442	40.596	10.028	1.00	49.88	C
ATOM	1414	O	ILE	A	180	11.018	40.531	8.878	1.00	50.41	O
ATOM	1415	CB	ILE	A	180	9.820	41.784	11.371	1.00	60.91	C
ATOM	1416	CG1	ILE	A	180	9.586	42.889	12.387	1.00	56.28	C
ATOM	1417	CG2	ILE	A	180	9.544	40.416	11.996	1.00	58.36	C
ATOM	1418	CD1	ILE	A	180	8.206	42.834	12.973	1.00	63.77	C
ATOM	1419	N	ASN	A	181	12.088	39.607	10.632	1.00	49.49	N
ATOM	1420	CA	ASN	A	181	12.269	38.308	10.010	1.00	44.31	C
ATOM	1421	C	ASN	A	181	12.329	37.382	11.223	1.00	53.84	C
ATOM	1422	O	ASN	A	181	12.789	37.776	12.297	1.00	49.42	O
ATOM	1423	CB	ASN	A	181	13.555	38.240	9.189	1.00	50.86	C
ATOM	1424	CG	ASN	A	181	13.527	37.117	8.165	1.00	58.63	C
ATOM	1425	OD1	ASN	A	181	12.581	36.332	8.126	1.00	68.55	O
ATOM	1426	ND2	ASN	A	181	14.567	37.031	7.331	1.00	62.99	N
ATOM	1427	N	PHE	A	182	11.818	36.172	11.082	1.00	51.66	N
ATOM	1428	CA	PHE	A	182	11.839	35.261	12.210	1.00	54.82	C
ATOM	1429	C	PHE	A	182	12.052	33.843	11.711	1.00	62.75	C
ATOM	1430	O	PHE	A	182	11.914	33.563	10.512	1.00	55.35	O
ATOM	1431	CB	PHE	A	182	10.521	35.354	12.989	1.00	62.28	C
ATOM	1432	CG	PHE	A	182	9.352	34.717	12.283	1.00	74.94	C
ATOM	1433	CD1	PHE	A	182	9.292	33.333	12.120	1.00	82.11	C
ATOM	1434	CD2	PHE	A	182	8.333	35.496	11.745	1.00	81.28	C
ATOM	1435	CE1	PHE	A	182	8.244	32.733	11.429	1.00	84.02	C
ATOM	1436	CE2	PHE	A	182	7.276	34.901	11.049	1.00	84.09	C
ATOM	1437	CZ	PHE	A	182	7.236	33.516	10.892	1.00	83.03	C
ATOM	1438	N	LYS	A	183	12.388	32.946	12.633	1.00	58.39	N
ATOM	1439	CA	LYS	A	183	12.591	31.541	12.295	1.00	50.63	C
ATOM	1440	C	LYS	A	183	12.106	30.678	13.459	1.00	53.23	C
ATOM	1441	O	LYS	A	183	12.431	30.947	14.622	1.00	45.57	O
ATOM	1442	CB	LYS	A	183	14.073	31.263	12.022	1.00	65.15	C
ATOM	1443	CG	LYS	A	183	14.446	29.780	11.957	1.00	64.65	C
ATOM	1444	CD	LYS	A	183	14.295	29.166	10.566	1.00	63.11	C
ATOM	1445	CE	LYS	A	183	14.627	27.670	10.590	1.00	53.42	C
ATOM	1446	NZ	LYS	A	183	15.665	27.264	9.599	1.00	53.61	N
ATOM	1447	N	ASP	A	184	11.319	29.655	13.142	1.00	48.66	N
ATOM	1448	CA	ASP	A	184	10.797	28.751	14.156	1.00	52.92	C
ATOM	1449	C	ASP	A	184	11.722	27.567	14.333	1.00	45.71	C
ATOM	1450	O	ASP	A	184	12.104	26.894	13.371	1.00	44.54	O
ATOM	1451	CB	ASP	A	184	9.404	28.255	13.784	1.00	62.54	C
ATOM	1452	CG	ASP	A	184	8.338	29.306	14.007	1.00	62.50	C
ATOM	1453	OD1	ASP	A	184	8.407	30.010	15.038	1.00	56.56	O
ATOM	1454	OD2	ASP	A	184	7.429	29.417	13.155	1.00	70.30	O
ATOM	1455	N	ILE	A	185	12.085	27.313	15.576	1.00	40.93	N
ATOM	1456	CA	ILE	A	185	12.993	26.219	15.849	1.00	39.71	C
ATOM	1457	C	ILE	A	185	12.372	25.231	16.806	1.00	38.52	C
ATOM	1458	O	ILE	A	185	11.958	25.590	17.909	1.00	38.65	O
ATOM	1459	CB	ILE	A	185	14.326	26.752	16.417	1.00	41.45	C
ATOM	1460	CG1	ILE	A	185	15.051	27.548	15.316	1.00	46.89	C
ATOM	1461	CG2	ILE	A	185	15.199	25.580	16.922	1.00	37.86	C
ATOM	1462	CD1	ILE	A	185	16.246	28.337	15.805	1.00	48.29	C
ATOM	1463	N	GLN	A	186	12.291	23.984	16.355	1.00	42.25	N
ATOM	1464	CA	GLN	A	186	11.744	22.916	17.181	1.00	41.47	C
ATOM	1465	C	GLN	A	186	12.857	22.416	18.097	1.00	38.63	C

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ATOM	1466	O	GLN	A	186	13.916	21.991	17.630	1.00	42.48	O
ATOM	1467	CB	GLN	A	186	11.247	21.755	16.307	1.00	52.01	C
ATOM	1468	CG	GLN	A	186	10.732	20.542	17.100	1.00	64.38	C
ATOM	1469	CD	GLN	A	186	10.353	19.348	16.204	1.00	79.51	C
ATOM	1470	OE1	GLN	A	186	10.873	19.202	15.092	1.00	79.17	O
ATOM	1471	NE2	GLN	A	186	9.465	18.481	16.701	1.00	80.31	N
ATOM	1472	N	VAL	A	187	12.610	22.457	19.398	1.00	43.44	N
ATOM	1473	CA	VAL	A	187	13.586	21.987	20.367	1.00	47.67	C
ATOM	1474	C	VAL	A	187	13.146	20.607	20.866	1.00	49.13	C
ATOM	1475	O	VAL	A	187	12.015	20.446	21.311	1.00	40.93	O
ATOM	1476	CB	VAL	A	187	13.675	22.939	21.583	1.00	42.03	C
ATOM	1477	CG1	VAL	A	187	14.563	22.315	22.652	1.00	41.16	C
ATOM	1478	CG2	VAL	A	187	14.224	24.300	21.154	1.00	38.03	C
ATOM	1479	N	ILE	A	188	14.035	19.621	20.785	1.00	41.32	N
ATOM	1480	CA	ILE	A	188	13.733	18.273	21.255	1.00	42.62	C
ATOM	1481	C	ILE	A	188	14.635	17.913	22.441	1.00	40.36	C
ATOM	1482	O	ILE	A	188	15.835	18.224	22.442	1.00	42.29	O
ATOM	1483	CB	ILE	A	188	13.945	17.213	20.142	1.00	45.03	C
ATOM	1484	CG1	ILE	A	188	13.002	17.475	18.967	1.00	41.79	C
ATOM	1485	CG2	ILE	A	188	13.687	15.806	20.702	1.00	46.59	C
ATOM	1486	CD1	ILE	A	188	13.267	16.566	17.763	1.00	40.92	C
ATOM	1487	N	VAL	A	189	14.050	17.285	23.455	1.00	36.36	N
ATOM	1488	CA	VAL	A	189	14.808	16.867	24.627	1.00	42.50	C
ATOM	1489	C	VAL	A	189	14.802	15.338	24.667	1.00	48.22	C
ATOM	1490	O	VAL	A	189	13.748	14.705	24.672	1.00	41.17	O
ATOM	1491	CB	VAL	A	189	14.206	17.455	25.921	1.00	44.30	C
ATOM	1492	CG1	VAL	A	189	14.945	16.930	27.125	1.00	39.49	C
ATOM	1493	CG2	VAL	A	189	14.304	18.966	25.894	1.00	40.56	C
ATOM	1494	N	ASN	A	190	15.993	14.754	24.665	1.00	40.63	N
ATOM	1495	CA	ASN	A	190	16.143	13.316	24.698	1.00	40.98	C
ATOM	1496	C	ASN	A	190	16.395	12.885	26.148	1.00	45.73	C
ATOM	1497	O	ASN	A	190	17.018	13.613	26.918	1.00	45.44	O
ATOM	1498	CB	ASN	A	190	17.285	12.908	23.752	1.00	40.78	C
ATOM	1499	CG	ASN	A	190	16.999	13.293	22.310	1.00	48.31	C
ATOM	1500	OD1	ASN	A	190	15.917	13.005	21.782	1.00	44.75	O
ATOM	1501	ND2	ASN	A	190	17.962	13.951	21.664	1.00	41.66	N
ATOM	1502	N	VAL	A	191	15.877	11.710	26.509	1.00	42.84	N
ATOM	1503	CA	VAL	A	191	15.982	11.151	27.863	1.00	39.39	C
ATOM	1504	C	VAL	A	191	16.683	9.802	27.788	1.00	39.64	C
ATOM	1505	O	VAL	A	191	16.261	8.910	27.043	1.00	47.40	O
ATOM	1506	CB	VAL	A	191	14.574	10.954	28.470	1.00	44.63	C
ATOM	1507	CG1	VAL	A	191	14.671	10.368	29.890	1.00	41.78	C
ATOM	1508	CG2	VAL	A	191	13.848	12.310	28.499	1.00	41.72	C
ATOM	1509	N	PRO	A	192	17.775	9.641	28.542	1.00	43.27	N
ATOM	1510	CA	PRO	A	192	18.578	8.416	28.596	1.00	45.21	C
ATOM	1511	C	PRO	A	192	17.722	7.224	28.990	1.00	42.00	C
ATOM	1512	O	PRO	A	192	16.783	7.355	29.763	1.00	42.35	O
ATOM	1513	CB	PRO	A	192	19.620	8.737	29.668	1.00	49.92	C
ATOM	1514	CG	PRO	A	192	19.690	10.204	29.687	1.00	49.81	C
ATOM	1515	CD	PRO	A	192	18.246	10.602	29.556	1.00	43.30	C
ATOM	1516	N	PRO	A	193	18.075	6.034	28.515	1.00	40.57	N
ATOM	1517	CA	PRO	A	193	17.301	4.848	28.838	1.00	39.79	C
ATOM	1518	C	PRO	A	193	17.516	4.372	30.256	1.00	43.45	C
ATOM	1519	O	PRO	A	193	18.552	4.666	30.864	1.00	44.20	O
ATOM	1520	CB	PRO	A	193	17.842	3.809	27.853	1.00	41.07	C
ATOM	1521	CG	PRO	A	193	18.661	4.630	26.843	1.00	46.01	C

Figure 2 (Table 2 (page 35))

ATOM	1522	CD	PRO	A	193	19.250	5.657	27.729	1.00	47.13	C
ATOM	1523	N	THR	A	194	16.516	3.665	30.779	1.00	45.04	N
ATOM	1524	CA	THR	A	194	16.614	2.987	32.075	1.00	48.33	C
ATOM	1525	C	THR	A	194	16.019	1.623	31.713	1.00	51.40	C
ATOM	1526	O	THR	A	194	15.124	1.529	30.848	1.00	41.84	O
ATOM	1527	CB	THR	A	194	15.792	3.630	33.225	1.00	48.61	C
ATOM	1528	OG1	THR	A	194	14.414	3.724	32.862	1.00	54.30	O
ATOM	1529	CG2	THR	A	194	16.338	4.992	33.574	1.00	57.24	C
ATOM	1530	N	VAL	A	195	16.507	0.565	32.352	1.00	48.50	N
ATOM	1531	CA	VAL	A	195	16.026	-0.760	32.017	1.00	45.60	C
ATOM	1532	C	VAL	A	195	16.083	-1.715	33.200	1.00	42.61	C
ATOM	1533	O	VAL	A	195	16.976	-1.644	34.021	1.00	46.25	O
ATOM	1534	CB	VAL	A	195	16.853	-1.346	30.840	1.00	42.93	C
ATOM	1535	CG1	VAL	A	195	18.314	-1.582	31.282	1.00	43.08	C
ATOM	1536	CG2	VAL	A	195	16.218	-2.635	30.339	1.00	43.46	C
ATOM	1537	N	GLN	A	196	15.104	-2.603	33.282	1.00	41.51	N
ATOM	1538	CA	GLN	A	196	15.070	-3.577	34.355	1.00	48.63	C
ATOM	1539	C	GLN	A	196	14.615	-4.928	33.817	1.00	46.66	C
ATOM	1540	O	GLN	A	196	13.706	-5.009	32.992	1.00	45.71	O
ATOM	1541	CB	GLN	A	196	14.119	-3.118	35.477	1.00	49.59	C
ATOM	1542	CG	GLN	A	196	14.693	-2.064	36.393	1.00	55.69	C
ATOM	1543	CD	GLN	A	196	13.790	-1.757	37.588	1.00	74.35	C
ATOM	1544	OE1	GLN	A	196	14.268	-1.328	38.639	1.00	74.51	O
ATOM	1545	NE2	GLN	A	196	12.482	-1.970	37.429	1.00	79.78	N
ATOM	1546	N	ALA	A	197	15.257	-5.991	34.282	1.00	40.70	N
ATOM	1547	CA	ALA	A	197	14.876	-7.329	33.873	1.00	39.75	C
ATOM	1548	C	ALA	A	197	13.550	-7.650	34.550	1.00	42.61	C
ATOM	1549	O	ALA	A	197	13.316	-7.246	35.687	1.00	48.54	O
ATOM	1550	CB	ALA	A	197	15.940	-8.333	34.313	1.00	39.72	C
ATOM	1551	N	ARG	A	198	12.671	-8.368	33.865	1.00	43.54	N
ATOM	1552	CA	ARG	A	198	11.403	-8.720	34.485	1.00	44.25	C
ATOM	1553	C	ARG	A	198	11.664	-9.866	35.479	1.00	53.02	C
ATOM	1554	O	ARG	A	198	11.018	-9.960	36.528	1.00	45.60	O
ATOM	1555	CB	ARG	A	198	10.392	-9.131	33.416	1.00	49.38	C
ATOM	1556	CG	ARG	A	198	8.967	-8.992	33.873	1.00	56.08	C
ATOM	1557	CD	ARG	A	198	7.991	-9.099	32.724	1.00	58.30	C
ATOM	1558	NE	ARG	A	198	7.873	-7.869	31.947	1.00	47.20	N
ATOM	1559	CZ	ARG	A	198	6.931	-7.675	31.030	1.00	54.23	C
ATOM	1560	NH1	ARG	A	198	6.038	-8.633	30.793	1.00	47.47	N
ATOM	1561	NH2	ARG	A	198	6.882	-6.541	30.339	1.00	50.85	N
ATOM	1562	N	GLN	A	199	12.625	-10.722	35.133	1.00	51.86	N
ATOM	1563	CA	GLN	A	199	13.047	-11.844	35.965	1.00	52.79	C
ATOM	1564	C	GLN	A	199	14.564	-11.926	35.871	1.00	50.17	C
ATOM	1565	O	GLN	A	199	15.107	-12.162	34.798	1.00	54.53	O
ATOM	1566	CB	GLN	A	199	12.447	-13.159	35.472	1.00	58.34	C
ATOM	1567	CG	GLN	A	199	10.941	-13.292	35.635	1.00	68.50	C
ATOM	1568	CD	GLN	A	199	10.498	-13.315	37.100	1.00	83.24	C
ATOM	1569	OE1	GLN	A	199	11.300	-13.596	37.996	1.00	85.74	O
ATOM	1570	NE2	GLN	A	199	9.214	-13.035	37.347	1.00	71.40	N
ATOM	1571	N	SER	A	200	15.247	-11.719	36.991	1.00	46.12	N
ATOM	1572	CA	SER	A	200	16.715	-11.753	37.042	1.00	50.15	C
ATOM	1573	C	SER	A	200	17.328	-13.157	37.004	1.00	47.60	C
ATOM	1574	O	SER	A	200	18.458	-13.350	36.541	1.00	49.49	O
ATOM	1575	CB	SER	A	200	17.194	-11.061	38.318	1.00	49.46	C
ATOM	1576	OG	SER	A	200	16.702	-9.737	38.384	1.00	76.11	O
ATOM	1577	N	ILE	A	201	16.576	-14.122	37.518	1.00	48.87	N

Figure 2 (Table 2 (page 36))

ATOM	1578	CA	ILE	A	201	17.019	-15.504	37.591	1.00	50.62	C
ATOM	1579	C	ILE	A	201	15.994	-16.400	36.925	1.00	47.35	C
ATOM	1580	O	ILE	A	201	14.797	-16.328	37.216	1.00	51.41	O
ATOM	1581	CB	ILE	A	201	17.181	-15.962	39.067	1.00	64.29	C
ATOM	1582	CG1	ILE	A	201	18.080	-14.983	39.838	1.00	57.76	C
ATOM	1583	CG2	ILE	A	201	17.768	-17.373	39.116	1.00	58.42	C
ATOM	1584	CD1	ILE	A	201	19.476	-14.860	39.290	1.00	68.87	C
ATOM	1585	N	VAL	A	202	16.469	-17.249	36.032	1.00	46.21	N
ATOM	1586	CA	VAL	A	202	15.587	-18.157	35.339	1.00	49.25	C
ATOM	1587	C	VAL	A	202	16.207	-19.540	35.336	1.00	47.17	C
ATOM	1588	O	VAL	A	202	17.391	-19.687	35.045	1.00	43.79	O
ATOM	1589	CB	VAL	A	202	15.371	-17.701	33.882	1.00	53.12	C
ATOM	1590	CG1	VAL	A	202	14.436	-18.661	33.177	1.00	45.19	C
ATOM	1591	CG2	VAL	A	202	14.820	-16.276	33.861	1.00	50.64	C
ATOM	1592	N	ASN	A	203	15.393	-20.544	35.653	1.00	49.57	N
ATOM	1593	CA	ASN	A	203	15.827	-21.937	35.680	1.00	51.28	C
ATOM	1594	C	ASN	A	203	15.078	-22.676	34.575	1.00	55.81	C
ATOM	1595	O	ASN	A	203	13.857	-22.541	34.440	1.00	50.57	O
ATOM	1596	CB	ASN	A	203	15.473	-22.635	37.010	1.00	49.03	C
ATOM	1597	CG	ASN	A	203	16.218	-22.067	38.217	1.00	47.83	C
ATOM	1598	OD1	ASN	A	203	17.319	-21.530	38.105	1.00	47.54	O
ATOM	1599	ND2	ASN	A	203	15.617	-22.217	39.390	1.00	44.22	N
ATOM	1600	N	ALA	A	204	15.811	-23.487	33.825	1.00	53.79	N
ATOM	1601	CA	ALA	A	204	15.249	-24.272	32.738	1.00	58.78	C
ATOM	1602	C	ALA	A	204	15.827	-25.683	32.730	1.00	59.86	C
ATOM	1603	O	ALA	A	204	16.909	-25.933	33.268	1.00	58.63	O
ATOM	1604	CB	ALA	A	204	15.541	-23.592	31.408	1.00	54.08	C
ATOM	1605	N	THR	A	205	15.088	-26.592	32.100	1.00	63.01	N
ATOM	1606	CA	THR	A	205	15.483	-27.989	31.966	1.00	62.26	C
ATOM	1607	C	THR	A	205	15.949	-28.248	30.546	1.00	59.60	C
ATOM	1608	O	THR	A	205	15.282	-27.874	29.579	1.00	57.70	O
ATOM	1609	CB	THR	A	205	14.323	-28.946	32.265	1.00	63.31	C
ATOM	1610	OG1	THR	A	205	13.916	-28.799	33.634	1.00	64.86	O
ATOM	1611	CG2	THR	A	205	14.760	-30.383	32.012	1.00	70.94	C
ATOM	1612	N	ALA	A	206	17.089	-28.913	30.430	1.00	56.34	N
ATOM	1613	CA	ALA	A	206	17.670	-29.203	29.134	1.00	60.33	C
ATOM	1614	C	ALA	A	206	17.035	-30.352	28.375	1.00	64.54	C
ATOM	1615	O	ALA	A	206	16.377	-31.228	28.940	1.00	68.98	O
ATOM	1616	CB	ALA	A	206	19.156	-29.464	29.290	1.00	58.07	C
ATOM	1617	N	ASN	A	207	17.246	-30.306	27.067	1.00	71.10	N
ATOM	1618	CA	ASN	A	207	16.791	-31.322	26.140	1.00	71.82	C
ATOM	1619	C	ASN	A	207	15.352	-31.788	26.216	1.00	70.92	C
ATOM	1620	O	ASN	A	207	15.077	-32.971	26.023	1.00	73.91	O
ATOM	1621	CB	ASN	A	207	17.724	-32.518	26.249	1.00	69.97	C
ATOM	1622	CG	ASN	A	207	19.170	-32.119	26.105	1.00	75.29	C
ATOM	1623	OD1	ASN	A	207	19.562	-31.531	25.097	1.00	81.94	O
ATOM	1624	ND2	ASN	A	207	19.972	-32.421	27.115	1.00	80.72	N
ATOM	1625	N	LEU	A	208	14.432	-30.877	26.496	1.00	67.07	N
ATOM	1626	CA	LEU	A	208	13.026	-31.246	26.528	1.00	68.52	C
ATOM	1627	C	LEU	A	208	12.347	-30.484	25.391	1.00	67.74	C
ATOM	1628	O	LEU	A	208	11.122	-30.415	25.306	1.00	73.14	O
ATOM	1629	CB	LEU	A	208	12.393	-30.904	27.877	1.00	68.09	C
ATOM	1630	CG	LEU	A	208	12.930	-31.679	29.091	1.00	79.90	C
ATOM	1631	CD1	LEU	A	208	12.105	-31.321	30.319	1.00	73.01	C
ATOM	1632	CD2	LEU	A	208	12.854	-33.180	28.843	1.00	77.54	C
ATOM	1633	N	GLY	A	209	13.175	-29.907	24.519	1.00	74.00	N

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ATOM	1634	CA	GLY	A	209	12.694	-29.159	23.364	1.00	81.72	C
ATOM	1635	C	GLY	A	209	11.907	-27.893	23.667	1.00	87.49	C
ATOM	1636	O	GLY	A	209	11.241	-27.341	22.788	1.00	95.12	O
ATOM	1637	N	GLN	A	210	11.992	-27.420	24.905	1.00	84.00	N
ATOM	1638	CA	GLN	A	210	11.254	-26.230	25.299	1.00	82.13	C
ATOM	1639	C	GLN	A	210	12.033	-24.922	25.205	1.00	74.00	C
ATOM	1640	O	GLN	A	210	13.265	-24.922	25.132	1.00	71.75	O
ATOM	1641	CB	GLN	A	210	10.703	-26.400	26.711	1.00	86.64	C
ATOM	1642	CG	GLN	A	210	11.770	-26.685	27.754	1.00	92.84	C
ATOM	1643	CD	GLN	A	210	11.215	-27.469	28.932	1.00	98.28	C
ATOM	1644	OE1	GLN	A	210	10.047	-27.856	28.930	1.00	102.57	O
ATOM	1645	NE2	GLN	A	210	12.049	-27.714	29.938	1.00	100.49	N
ATOM	1646	N	SER	A	211	11.295	-23.810	25.212	1.00	73.42	N
ATOM	1647	CA	SER	A	211	11.873	-22.470	25.101	1.00	68.89	C
ATOM	1648	C	SER	A	211	11.749	-21.688	26.394	1.00	59.63	C
ATOM	1649	O	SER	A	211	10.995	-22.044	27.297	1.00	58.00	O
ATOM	1650	CB	SER	A	211	11.181	-21.680	23.978	1.00	69.06	C
ATOM	1651	OG	SER	A	211	11.312	-22.319	22.719	1.00	75.29	O
ATOM	1652	N	VAL	A	212	12.515	-20.616	26.479	1.00	62.83	N
ATOM	1653	CA	VAL	A	212	12.470	-19.749	27.638	1.00	57.69	C
ATOM	1654	C	VAL	A	212	12.482	-18.343	27.056	1.00	51.71	C
ATOM	1655	O	VAL	A	212	13.140	-18.086	26.044	1.00	48.36	O
ATOM	1656	CB	VAL	A	212	13.697	-19.965	28.554	1.00	58.76	C
ATOM	1657	CG1	VAL	A	212	14.970	-19.802	27.762	1.00	57.99	C
ATOM	1658	CG2	VAL	A	212	13.665	-18.988	29.707	1.00	65.40	C
ATOM	1659	N	THR	A	213	11.738	-17.438	27.672	1.00	48.53	N
ATOM	1660	CA	THR	A	213	11.698	-16.079	27.171	1.00	50.94	C
ATOM	1661	C	THR	A	213	12.279	-15.100	28.194	1.00	46.89	C
ATOM	1662	O	THR	A	213	11.760	-14.969	29.301	1.00	48.85	O
ATOM	1663	CB	THR	A	213	10.246	-15.669	26.820	1.00	50.59	C
ATOM	1664	OG1	THR	A	213	9.720	-16.556	25.827	1.00	54.06	O
ATOM	1665	CG2	THR	A	213	10.214	-14.255	26.276	1.00	56.06	C
ATOM	1666	N	LEU	A	214	13.367	-14.430	27.823	1.00	50.67	N
ATOM	1667	CA	LEU	A	214	14.015	-13.445	28.686	1.00	44.75	C
ATOM	1668	C	LEU	A	214	13.444	-12.078	28.327	1.00	49.46	C
ATOM	1669	O	LEU	A	214	13.339	-11.738	27.147	1.00	40.16	O
ATOM	1670	CB	LEU	A	214	15.519	-13.469	28.464	1.00	40.05	C
ATOM	1671	CG	LEU	A	214	16.140	-14.857	28.611	1.00	47.06	C
ATOM	1672	CD1	LEU	A	214	17.647	-14.728	28.666	1.00	41.62	C
ATOM	1673	CD2	LEU	A	214	15.623	-15.532	29.880	1.00	42.47	C
ATOM	1674	N	VAL	A	215	13.089	-11.299	29.345	1.00	44.86	N
ATOM	1675	CA	VAL	A	215	12.454	-10.004	29.143	1.00	46.92	C
ATOM	1676	C	VAL	A	215	13.030	-8.850	29.928	1.00	48.90	C
ATOM	1677	O	VAL	A	215	13.254	-8.937	31.135	1.00	50.91	O
ATOM	1678	CB	VAL	A	215	10.969	-10.089	29.508	1.00	49.64	C
ATOM	1679	CG1	VAL	A	215	10.265	-8.759	29.213	1.00	50.90	C
ATOM	1680	CG2	VAL	A	215	10.332	-11.234	28.765	1.00	52.37	C
ATOM	1681	N	CYS	A	216	13.254	-7.755	29.221	1.00	44.39	N
ATOM	1682	CA	CYS	A	216	13.754	-6.542	29.826	1.00	45.29	C
ATOM	1683	C	CYS	A	216	12.744	-5.449	29.501	1.00	52.26	C
ATOM	1684	O	CYS	A	216	12.223	-5.399	28.393	1.00	47.28	O
ATOM	1685	CB	CYS	A	216	15.122	-6.180	29.257	1.00	45.92	C
ATOM	1686	SG	CYS	A	216	16.483	-7.140	29.998	1.00	51.48	S
ATOM	1687	N	ASP	A	217	12.454	-4.598	30.478	1.00	44.49	N
ATOM	1688	CA	ASP	A	217	11.523	-3.499	30.291	1.00	46.18	C
ATOM	1689	C	ASP	A	217	12.330	-2.230	30.313	1.00	46.02	C

Figure 2 (Table 2 (page 38))

ATOM	1690	O	ASP	A	217	12.974	-1.906	31.307	1.00	42.34	O
ATOM	1691	CB	ASP	A	217	10.501	-3.453	31.419	1.00	43.07	C
ATOM	1692	CG	ASP	A	217	9.576	-4.624	31.382	1.00	54.67	C
ATOM	1693	OD1	ASP	A	217	8.860	-4.755	30.366	1.00	54.44	O
ATOM	1694	OD2	ASP	A	217	9.573	-5.417	32.350	1.00	52.78	O
ATOM	1695	N	ALA	A	218	12.279	-1.498	29.215	1.00	43.43	N
ATOM	1696	CA	ALA	A	218	13.030	-0.269	29.129	1.00	51.56	C
ATOM	1697	C	ALA	A	218	12.205	0.900	28.633	1.00	51.78	C
ATOM	1698	O	ALA	A	218	11.150	0.731	28.031	1.00	48.04	O
ATOM	1699	CB	ALA	A	218	14.221	-0.468	28.202	1.00	46.61	C
ATOM	1700	N	ASP	A	219	12.704	2.096	28.901	1.00	47.98	N
ATOM	1701	CA	ASP	A	219	12.076	3.287	28.377	1.00	53.40	C
ATOM	1702	C	ASP	A	219	13.097	4.412	28.287	1.00	54.39	C
ATOM	1703	O	ASP	A	219	14.214	4.308	28.791	1.00	53.10	O
ATOM	1704	CB	ASP	A	219	10.876	3.693	29.214	1.00	67.27	C
ATOM	1705	CG	ASP	A	219	11.226	3.878	30.644	1.00	73.00	C
ATOM	1706	OD1	ASP	A	219	12.424	4.087	30.905	1.00	77.65	O
ATOM	1707	OD2	ASP	A	219	10.315	3.824	31.502	1.00	83.21	O
ATOM	1708	N	GLY	A	220	12.693	5.482	27.622	1.00	46.12	N
ATOM	1709	CA	GLY	A	220	13.541	6.632	27.405	1.00	43.59	C
ATOM	1710	C	GLY	A	220	13.035	7.286	26.135	1.00	46.49	C
ATOM	1711	O	GLY	A	220	12.062	6.810	25.554	1.00	45.48	O
ATOM	1712	N	PHE	A	221	13.700	8.341	25.678	1.00	43.50	N
ATOM	1713	CA	PHE	A	221	13.283	9.017	24.465	1.00	42.29	C
ATOM	1714	C	PHE	A	221	14.499	9.499	23.669	1.00	33.90	C
ATOM	1715	O	PHE	A	221	15.313	10.265	24.178	1.00	43.58	O
ATOM	1716	CB	PHE	A	221	12.391	10.215	24.797	1.00	41.04	C
ATOM	1717	CG	PHE	A	221	11.792	10.861	23.572	1.00	44.52	C
ATOM	1718	CD1	PHE	A	221	10.591	10.395	23.037	1.00	47.33	C
ATOM	1719	CD2	PHE	A	221	12.482	11.863	22.891	1.00	44.34	C
ATOM	1720	CE1	PHE	A	221	10.088	10.910	21.837	1.00	45.26	C
ATOM	1721	CE2	PHE	A	221	11.989	12.380	21.693	1.00	48.97	C
ATOM	1722	CZ	PHE	A	221	10.785	11.897	21.166	1.00	44.61	C
ATOM	1723	N	PRO	A	222	14.645	9.050	22.400	1.00	40.11	N
ATOM	1724	CA	PRO	A	222	13.780	8.122	21.655	1.00	40.06	C
ATOM	1725	C	PRO	A	222	13.693	6.765	22.344	1.00	50.45	C
ATOM	1726	O	PRO	A	222	14.546	6.419	23.172	1.00	43.37	O
ATOM	1727	CB	PRO	A	222	14.480	8.000	20.307	1.00	44.90	C
ATOM	1728	CG	PRO	A	222	15.163	9.311	20.158	1.00	43.89	C
ATOM	1729	CD	PRO	A	222	15.733	9.547	21.536	1.00	38.16	C
ATOM	1730	N	GLU	A	223	12.659	5.999	21.998	1.00	47.32	N
ATOM	1731	CA	GLU	A	223	12.466	4.664	22.565	1.00	48.48	C
ATOM	1732	C	GLU	A	223	13.778	3.917	22.403	1.00	44.89	C
ATOM	1733	O	GLU	A	223	14.364	3.886	21.321	1.00	42.04	O
ATOM	1734	CB	GLU	A	223	11.359	3.905	21.837	1.00	51.24	C
ATOM	1735	CG	GLU	A	223	9.947	4.402	22.100	1.00	45.06	C
ATOM	1736	CD	GLU	A	223	9.513	4.303	23.556	1.00	60.54	C
ATOM	1737	OE1	GLU	A	223	9.950	3.368	24.263	1.00	71.83	O
ATOM	1738	OE2	GLU	A	223	8.700	5.153	23.986	1.00	70.97	O
ATOM	1739	N	PRO	A	224	14.249	3.296	23.483	1.00	46.34	N
ATOM	1740	CA	PRO	A	224	15.507	2.559	23.453	1.00	48.92	C
ATOM	1741	C	PRO	A	224	15.536	1.373	22.501	1.00	49.30	C
ATOM	1742	O	PRO	A	224	14.535	0.692	22.311	1.00	47.42	O
ATOM	1743	CB	PRO	A	224	15.678	2.113	24.911	1.00	47.68	C
ATOM	1744	CG	PRO	A	224	14.893	3.128	25.698	1.00	57.81	C
ATOM	1745	CD	PRO	A	224	13.673	3.314	24.843	1.00	47.48	C

Figure 2 (Table 2 (page 39))

ATOM	1746	N	THR	A	225	16.685	1.143	21.884	1.00	50.13	N
ATOM	1747	CA	THR	A	225	16.859	-0.016	21.021	1.00	60.61	C
ATOM	1748	C	THR	A	225	17.598	-1.033	21.907	1.00	59.15	C
ATOM	1749	O	THR	A	225	18.533	-0.663	22.631	1.00	47.10	O
ATOM	1750	CB	THR	A	225	17.723	0.319	19.810	1.00	58.08	C
ATOM	1751	OG1	THR	A	225	17.027	1.259	18.985	1.00	83.82	O
ATOM	1752	CG2	THR	A	225	18.009	-0.934	19.003	1.00	73.24	C
ATOM	1753	N	MET	A	226	17.189	-2.296	21.862	1.00	52.21	N
ATOM	1754	CA	MET	A	226	17.824	-3.310	22.692	1.00	53.46	C
ATOM	1755	C	MET	A	226	18.721	-4.265	21.927	1.00	56.38	C
ATOM	1756	O	MET	A	226	18.417	-4.657	20.802	1.00	51.69	O
ATOM	1757	CB	MET	A	226	16.766	-4.149	23.397	1.00	61.02	C
ATOM	1758	CG	MET	A	226	15.711	-3.339	24.112	1.00	73.13	C
ATOM	1759	SD	MET	A	226	16.515	-2.409	25.388	1.00	79.72	S
ATOM	1760	CE	MET	A	226	17.052	-3.791	26.474	1.00	72.80	C
ATOM	1761	N	SER	A	227	19.821	-4.649	22.564	1.00	51.74	N
ATOM	1762	CA	SER	A	227	20.755	-5.617	22.003	1.00	57.86	C
ATOM	1763	C	SER	A	227	21.169	-6.496	23.187	1.00	61.93	C
ATOM	1764	O	SER	A	227	21.204	-6.024	24.332	1.00	60.05	O
ATOM	1765	CB	SER	A	227	21.961	-4.912	21.403	1.00	41.57	C
ATOM	1766	OG	SER	A	227	22.546	-4.056	22.355	1.00	62.88	O
ATOM	1767	N	TRP	A	228	21.472	-7.765	22.924	1.00	57.15	N
ATOM	1768	CA	TRP	A	228	21.840	-8.689	23.998	1.00	55.47	C
ATOM	1769	C	TRP	A	228	23.243	-9.290	23.899	1.00	59.04	C
ATOM	1770	O	TRP	A	228	23.856	-9.273	22.829	1.00	49.40	O
ATOM	1771	CB	TRP	A	228	20.842	-9.840	24.050	1.00	49.35	C
ATOM	1772	CG	TRP	A	228	19.435	-9.439	24.308	1.00	47.96	C
ATOM	1773	CD1	TRP	A	228	18.630	-8.695	23.494	1.00	53.38	C
ATOM	1774	CD2	TRP	A	228	18.654	-9.760	25.462	1.00	47.76	C
ATOM	1775	NE1	TRP	A	228	17.394	-8.537	24.067	1.00	52.08	N
ATOM	1776	CE2	TRP	A	228	17.379	-9.177	25.279	1.00	45.77	C
ATOM	1777	CE3	TRP	A	228	18.906	-10.482	26.637	1.00	42.71	C
ATOM	1778	CZ2	TRP	A	228	16.355	-9.291	26.227	1.00	37.55	C
ATOM	1779	CZ3	TRP	A	228	17.887	-10.598	27.586	1.00	45.83	C
ATOM	1780	CH2	TRP	A	228	16.625	-10.004	27.373	1.00	50.85	C
ATOM	1781	N	THR	A	229	23.749	-9.795	25.027	1.00	58.07	N
ATOM	1782	CA	THR	A	229	25.047	-10.474	25.057	1.00	60.10	C
ATOM	1783	C	THR	A	229	24.918	-11.741	25.902	1.00	61.83	C
ATOM	1784	O	THR	A	229	24.132	-11.787	26.868	1.00	54.86	O
ATOM	1785	CB	THR	A	229	26.191	-9.610	25.652	1.00	53.98	C
ATOM	1786	OG1	THR	A	229	25.882	-9.252	26.999	1.00	57.01	O
ATOM	1787	CG2	THR	A	229	26.418	-8.373	24.816	1.00	57.89	C
ATOM	1788	N	LYS	A	230	25.677	-12.765	25.515	1.00	58.82	N
ATOM	1789	CA	LYS	A	230	25.684	-14.043	26.217	1.00	58.37	C
ATOM	1790	C	LYS	A	230	27.088	-14.147	26.792	1.00	52.83	C
ATOM	1791	O	LYS	A	230	28.066	-14.266	26.054	1.00	54.49	O
ATOM	1792	CB	LYS	A	230	25.396	-15.173	25.227	1.00	55.01	C
ATOM	1793	CG	LYS	A	230	25.113	-16.539	25.849	1.00	45.56	C
ATOM	1794	CD	LYS	A	230	24.973	-17.615	24.757	1.00	59.41	C
ATOM	1795	CE	LYS	A	230	24.803	-19.019	25.339	1.00	62.34	C
ATOM	1796	NZ	LYS	A	230	24.460	-20.050	24.304	1.00	59.23	N
ATOM	1797	N	ASP	A	231	27.183	-14.078	28.115	1.00	61.62	N
ATOM	1798	CA	ASP	A	231	28.479	-14.105	28.781	1.00	69.33	C
ATOM	1799	C	ASP	A	231	29.439	-13.118	28.113	1.00	69.66	C
ATOM	1800	O	ASP	A	231	30.612	-13.429	27.916	1.00	73.37	O
ATOM	1801	CB	ASP	A	231	29.096	-15.509	28.754	1.00	67.95	C



Figure 2 (Table 2 (page 40))

ATOM	1802	CG	ASP	A	231	28.359	-16.492	29.645	1.00	76.63	C
ATOM	1803	OD1	ASP	A	231	27.830	-16.069	30.697	1.00	73.37	O
ATOM	1804	OD2	ASP	A	231	28.327	-17.692	29.295	1.00	73.07	O
ATOM	1805	N	GLY	A	232	28.939	-11.933	27.766	1.00	69.81	N
ATOM	1806	CA	GLY	A	232	29.780	-10.925	27.147	1.00	62.92	C
ATOM	1807	C	GLY	A	232	29.815	-10.953	25.633	1.00	57.21	C
ATOM	1808	O	GLY	A	232	30.217	-9.985	24.999	1.00	64.11	O
ATOM	1809	N	GLU	A	233	29.398	-12.058	25.039	1.00	60.24	N
ATOM	1810	CA	GLU	A	233	29.407	-12.163	23.587	1.00	67.77	C
ATOM	1811	C	GLU	A	233	28.086	-11.753	22.977	1.00	69.76	C
ATOM	1812	O	GLU	A	233	27.019	-12.146	23.437	1.00	67.85	O
ATOM	1813	CB	GLU	A	233	29.721	-13.589	23.156	1.00	73.47	C
ATOM	1814	CG	GLU	A	233	31.174	-13.980	23.298	1.00	93.05	C
ATOM	1815	CD	GLU	A	233	32.100	-13.154	22.416	1.00	101.69	C
ATOM	1816	OE1	GLU	A	233	31.753	-12.894	21.241	1.00	104.10	O
ATOM	1817	OE2	GLU	A	233	33.189	-12.771	22.898	1.00	105.15	O
ATOM	1818	N	PRO	A	234	28.146	-10.986	21.894	1.00	69.71	N
ATOM	1819	CA	PRO	A	234	26.928	-10.527	21.227	1.00	69.07	C
ATOM	1820	C	PRO	A	234	26.042	-11.660	20.747	1.00	63.95	C
ATOM	1821	O	PRO	A	234	26.516	-12.774	20.513	1.00	68.33	O
ATOM	1822	CB	PRO	A	234	27.463	-9.717	20.047	1.00	74.23	C
ATOM	1823	CG	PRO	A	234	28.863	-9.346	20.458	1.00	78.24	C
ATOM	1824	CD	PRO	A	234	29.349	-10.575	21.151	1.00	73.22	C
ATOM	1825	N	ILE	A	235	24.756	-11.361	20.589	1.00	60.42	N
ATOM	1826	CA	ILE	A	235	23.819	-12.347	20.075	1.00	59.30	C
ATOM	1827	C	ILE	A	235	23.091	-11.707	18.887	1.00	73.94	C
ATOM	1828	O	ILE	A	235	22.292	-10.780	19.062	1.00	69.18	O
ATOM	1829	CB	ILE	A	235	22.785	-12.748	21.118	1.00	58.75	C
ATOM	1830	CG1	ILE	A	235	23.480	-13.103	22.435	1.00	60.61	C
ATOM	1831	CG2	ILE	A	235	21.986	-13.935	20.602	1.00	54.52	C
ATOM	1832	CD1	ILE	A	235	22.535	-13.237	23.598	1.00	58.31	C
ATOM	1833	N	GLU	A	236	23.341	-12.205	17.679	1.00	80.94	N
ATOM	1834	CA	GLU	A	236	22.742	-11.605	16.488	1.00	90.13	C
ATOM	1835	C	GLU	A	236	21.234	-11.755	16.308	1.00	93.13	C
ATOM	1836	O	GLU	A	236	20.685	-12.857	16.339	1.00	89.58	O
ATOM	1837	CB	GLU	A	236	23.493	-12.094	15.252	1.00	98.19	C
ATOM	1838	CG	GLU	A	236	25.017	-12.039	15.429	1.00	107.77	C
ATOM	1839	CD	GLU	A	236	25.542	-10.662	15.844	1.00	115.02	C
ATOM	1840	OE1	GLU	A	236	24.988	-10.055	16.788	1.00	121.81	O
ATOM	1841	OE2	GLU	A	236	26.526	-10.191	15.233	1.00	116.63	O
ATOM	1842	N	ASN	A	237	20.585	-10.606	16.115	1.00	98.73	N
ATOM	1843	CA	ASN	A	237	19.136	-10.494	15.944	1.00	104.56	C
ATOM	1844	C	ASN	A	237	18.609	-11.196	14.686	1.00	110.81	C
ATOM	1845	O	ASN	A	237	17.530	-11.792	14.705	1.00	112.81	O
ATOM	1846	CB	ASN	A	237	18.759	-9.004	15.930	1.00	100.46	C
ATOM	1847	CG	ASN	A	237	17.268	-8.761	16.142	1.00	100.48	C
ATOM	1848	OD1	ASN	A	237	16.868	-7.689	16.600	1.00	96.36	O
ATOM	1849	ND2	ASN	A	237	16.443	-9.747	15.798	1.00	97.08	N
ATOM	1850	N	GLU	A	238	19.382	-11.111	13.607	1.00	114.86	N
ATOM	1851	CA	GLU	A	238	19.072	-11.709	12.303	1.00	120.04	C
ATOM	1852	C	GLU	A	238	17.688	-12.328	12.095	1.00	121.21	C
ATOM	1853	O	GLU	A	238	16.975	-11.855	11.181	1.00	121.72	O
ATOM	1854	CB	GLU	A	238	20.152	-12.736	11.963	1.00	121.17	C
ATOM	1855	CG	GLU	A	238	21.557	-12.228	12.238	1.00	126.14	C
ATOM	1856	CD	GLU	A	238	21.808	-10.840	11.662	1.00	130.48	C
ATOM	1857	OE1	GLU	A	238	21.090	-9.885	12.034	1.00	132.56	O

Figure 2 (Table 2 (page 41))

ATOM	1858	OE2	GLU	A	238	22.731	-10.705	10.837	1.00134.55	O
ATOM	1859	N	ASP	A	241	18.070	-14.713	9.305	1.00127.03	N
ATOM	1860	CA	ASP	A	241	17.685	-16.080	9.767	1.00127.98	C
ATOM	1861	C	ASP	A	241	17.960	-16.274	11.255	1.00129.18	C
ATOM	1862	O	ASP	A	241	18.938	-15.754	11.803	1.00129.01	O
ATOM	1863	CB	ASP	A	241	18.443	-17.152	8.972	1.00124.42	C
ATOM	1864	CG	ASP	A	241	18.044	-18.574	9.365	1.00123.20	C
ATOM	1865	OD1	ASP	A	241	18.114	-18.916	10.570	1.00119.17	O
ATOM	1866	OD2	ASP	A	241	17.664	-19.356	8.464	1.00120.27	O
ATOM	1867	N	ASP	A	242	17.080	-17.043	11.888	1.00129.87	N
ATOM	1868	CA	ASP	A	242	17.157	-17.357	13.310	1.00128.52	C
ATOM	1869	C	ASP	A	242	16.420	-18.676	13.544	1.00124.12	C
ATOM	1870	O	ASP	A	242	15.291	-18.851	13.081	1.00127.28	O
ATOM	1871	CB	ASP	A	242	16.509	-16.230	14.128	1.00134.37	C
ATOM	1872	CG	ASP	A	242	15.076	-15.931	13.693	1.00137.89	C
ATOM	1873	OD1	ASP	A	242	14.695	-16.306	12.560	1.00139.91	O
ATOM	1874	OD2	ASP	A	242	14.335	-15.302	14.484	1.00138.48	O
ATOM	1875	N	GLU	A	243	17.053	-19.614	14.237	1.00115.47	N
ATOM	1876	CA	GLU	A	243	16.401	-20.892	14.492	1.00108.81	C
ATOM	1877	C	GLU	A	243	16.219	-21.065	15.984	1.00101.77	C
ATOM	1878	O	GLU	A	243	15.232	-21.637	16.453	1.00 97.50	O
ATOM	1879	CB	GLU	A	243	17.243	-22.056	13.957	1.00113.03	C
ATOM	1880	CG	GLU	A	243	18.587	-22.269	14.665	1.00119.77	C
ATOM	1881	CD	GLU	A	243	19.736	-21.500	14.022	1.00123.96	C
ATOM	1882	OE1	GLU	A	243	20.004	-21.723	12.821	1.00128.49	O
ATOM	1883	OE2	GLU	A	243	20.380	-20.682	14.716	1.00125.21	O
ATOM	1884	N	LYS	A	244	17.193	-20.552	16.719	1.00 90.55	N
ATOM	1885	CA	LYS	A	244	17.196	-20.652	18.159	1.00 87.36	C
ATOM	1886	C	LYS	A	244	16.847	-19.342	18.851	1.00 78.94	C
ATOM	1887	O	LYS	A	244	15.944	-19.299	19.681	1.00 79.48	O
ATOM	1888	CB	LYS	A	244	18.567	-21.157	18.623	1.00 85.94	C
ATOM	1889	CG	LYS	A	244	18.973	-20.687	20.009	1.00 90.77	C
ATOM	1890	CD	LYS	A	244	20.222	-21.392	20.527	1.00 85.35	C
ATOM	1891	CE	LYS	A	244	19.960	-22.872	20.764	1.00 85.15	C
ATOM	1892	NZ	LYS	A	244	18.698	-23.096	21.533	1.00 79.01	N
ATOM	1893	N	HIS	A	245	17.566	-18.279	18.510	1.00 72.67	N
ATOM	1894	CA	HIS	A	245	17.332	-16.978	19.121	1.00 73.65	C
ATOM	1895	C	HIS	A	245	16.275	-16.150	18.398	1.00 71.43	C
ATOM	1896	O	HIS	A	245	16.483	-15.726	17.264	1.00 73.85	O
ATOM	1897	CB	HIS	A	245	18.636	-16.191	19.174	1.00 62.45	C
ATOM	1898	CG	HIS	A	245	19.712	-16.860	19.968	1.00 73.56	C
ATOM	1899	ND1	HIS	A	245	19.566	-17.183	21.301	1.00 75.57	N
ATOM	1900	CD2	HIS	A	245	20.963	-17.251	19.624	1.00 74.25	C
ATOM	1901	CE1	HIS	A	245	20.680	-17.740	21.742	1.00 69.91	C
ATOM	1902	NE2	HIS	A	245	21.542	-17.792	20.747	1.00 78.21	N
ATOM	1903	N	ILE	A	246	15.151	-15.907	19.066	1.00 71.28	N
ATOM	1904	CA	ILE	A	246	14.061	-15.117	18.492	1.00 67.47	C
ATOM	1905	C	ILE	A	246	13.820	-13.823	19.279	1.00 68.54	C
ATOM	1906	O	ILE	A	246	13.465	-13.871	20.459	1.00 56.11	O
ATOM	1907	CB	ILE	A	246	12.746	-15.912	18.494	1.00 71.39	C
ATOM	1908	CG1	ILE	A	246	12.953	-17.270	17.829	1.00 73.66	C
ATOM	1909	CG2	ILE	A	246	11.656	-15.114	17.803	1.00 69.42	C
ATOM	1910	CD1	ILE	A	246	13.544	-17.182	16.451	1.00 82.71	C
ATOM	1911	N	PHE	A	247	13.991	-12.675	18.625	1.00 57.64	N
ATOM	1912	CA	PHE	A	247	13.783	-11.395	19.286	1.00 57.66	C
ATOM	1913	C	PHE	A	247	12.444	-10.766	19.000	1.00 59.75	C

Figure 2 (Table 2 (page 42))

ATOM	1914	O	PHE	A	247	11.842	-11.003	17.955	1.00	71.91	O
ATOM	1915	CB	PHE	A	247	14.831	-10.386	18.866	1.00	58.61	C
ATOM	1916	CG	PHE	A	247	16.205	-10.761	19.252	1.00	55.18	C
ATOM	1917	CD1	PHE	A	247	16.931	-11.663	18.486	1.00	63.52	C
ATOM	1918	CD2	PHE	A	247	16.791	-10.195	20.375	1.00	64.94	C
ATOM	1919	CE1	PHE	A	247	18.233	-11.994	18.836	1.00	56.98	C
ATOM	1920	CE2	PHE	A	247	18.084	-10.515	20.735	1.00	62.89	C
ATOM	1921	CZ	PHE	A	247	18.813	-11.416	19.963	1.00	69.14	C
ATOM	1922	N	SER	A	248	11.984	-9.948	19.939	1.00	60.62	N
ATOM	1923	CA	SER	A	248	10.741	-9.211	19.761	1.00	59.42	C
ATOM	1924	C	SER	A	248	11.135	-8.035	18.848	1.00	58.07	C
ATOM	1925	O	SER	A	248	12.324	-7.793	18.605	1.00	50.63	O
ATOM	1926	CB	SER	A	248	10.238	-8.684	21.107	1.00	51.67	C
ATOM	1927	OG	SER	A	248	11.212	-7.849	21.713	1.00	56.47	O
ATOM	1928	N	ASP	A	249	10.156	-7.286	18.364	1.00	62.87	N
ATOM	1929	CA	ASP	A	249	10.433	-6.168	17.461	1.00	68.58	C
ATOM	1930	C	ASP	A	249	11.414	-5.157	18.016	1.00	71.42	C
ATOM	1931	O	ASP	A	249	12.289	-4.649	17.304	1.00	70.32	O
ATOM	1932	CB	ASP	A	249	9.113	-5.519	17.102	1.00	78.97	C
ATOM	1933	CG	ASP	A	249	8.122	-6.538	16.598	1.00	85.41	C
ATOM	1934	OD1	ASP	A	249	8.266	-6.986	15.438	1.00	90.50	O
ATOM	1935	OD2	ASP	A	249	7.218	-6.926	17.370	1.00	85.77	O
ATOM	1936	N	ASP	A	250	11.274	-4.875	19.297	1.00	71.27	N
ATOM	1937	CA	ASP	A	250	12.159	-3.942	19.964	1.00	74.17	C
ATOM	1938	C	ASP	A	250	13.358	-4.713	20.521	1.00	70.10	C
ATOM	1939	O	ASP	A	250	14.337	-4.113	20.971	1.00	70.84	O
ATOM	1940	CB	ASP	A	250	11.390	-3.284	21.100	1.00	82.42	C
ATOM	1941	CG	ASP	A	250	10.583	-4.296	21.895	1.00	86.25	C
ATOM	1942	OD1	ASP	A	250	10.204	-5.350	21.328	1.00	87.71	O
ATOM	1943	OD2	ASP	A	250	10.316	-4.044	23.082	1.00	99.42	O
ATOM	1944	N	SER	A	251	13.266	-6.044	20.478	1.00	61.34	N
ATOM	1945	CA	SER	A	251	14.301	-6.932	21.005	1.00	60.93	C
ATOM	1946	C	SER	A	251	14.357	-6.787	22.529	1.00	55.43	C
ATOM	1947	O	SER	A	251	15.398	-6.997	23.149	1.00	54.55	O
ATOM	1948	CB	SER	A	251	15.667	-6.615	20.386	1.00	56.47	C
ATOM	1949	OG	SER	A	251	15.608	-6.719	18.971	1.00	68.26	O
ATOM	1950	N	SER	A	252	13.222	-6.419	23.120	1.00	44.12	N
ATOM	1951	CA	SER	A	252	13.132	-6.262	24.565	1.00	54.67	C
ATOM	1952	C	SER	A	252	12.961	-7.666	25.142	1.00	45.19	C
ATOM	1953	O	SER	A	252	13.231	-7.900	26.321	1.00	45.23	O
ATOM	1954	CB	SER	A	252	11.948	-5.359	24.957	1.00	50.26	C
ATOM	1955	OG	SER	A	252	10.705	-6.019	24.785	1.00	68.26	O
ATOM	1956	N	GLU	A	253	12.511	-8.586	24.288	1.00	39.14	N
ATOM	1957	CA	GLU	A	253	12.351	-9.984	24.655	1.00	42.86	C
ATOM	1958	C	GLU	A	253	13.245	-10.847	23.787	1.00	55.42	C
ATOM	1959	O	GLU	A	253	13.322	-10.649	22.573	1.00	55.46	O
ATOM	1960	CB	GLU	A	253	10.924	-10.475	24.459	1.00	46.35	C
ATOM	1961	CG	GLU	A	253	9.898	-9.823	25.335	1.00	52.21	C
ATOM	1962	CD	GLU	A	253	8.629	-10.640	25.406	1.00	55.68	C
ATOM	1963	OE1	GLU	A	253	8.464	-11.550	24.569	1.00	60.84	O
ATOM	1964	OE2	GLU	A	253	7.792	-10.370	26.296	1.00	63.61	O
ATOM	1965	N	LEU	A	254	13.925	-11.798	24.423	1.00	49.11	N
ATOM	1966	CA	LEU	A	254	14.793	-12.741	23.730	1.00	43.78	C
ATOM	1967	C	LEU	A	254	14.260	-14.129	24.052	1.00	54.16	C
ATOM	1968	O	LEU	A	254	14.179	-14.516	25.221	1.00	49.96	O
ATOM	1969	CB	LEU	A	254	16.240	-12.617	24.212	1.00	48.13	C

Figure 2 (Table 2 (page 43))

ATOM	1970	CG	LEU	A	254	17.132	-13.793	23.786	1.00	61.15	C
ATOM	1971	CD1	LEU	A	254	17.129	-13.902	22.264	1.00	56.30	C
ATOM	1972	CD2	LEU	A	254	18.561	-13.622	24.314	1.00	45.18	C
ATOM	1973	N	THR	A	255	13.874	-14.873	23.024	1.00	52.09	N
ATOM	1974	CA	THR	A	255	13.343	-16.214	23.233	1.00	55.30	C
ATOM	1975	C	THR	A	255	14.371	-17.254	22.822	1.00	57.05	C
ATOM	1976	O	THR	A	255	14.809	-17.279	21.677	1.00	56.25	O
ATOM	1977	CB	THR	A	255	12.050	-16.444	22.419	1.00	62.05	C
ATOM	1978	OG1	THR	A	255	10.999	-15.630	22.951	1.00	66.84	O
ATOM	1979	CG2	THR	A	255	11.625	-17.908	22.491	1.00	69.28	C
ATOM	1980	N	ILE	A	256	14.784	-18.085	23.774	1.00	57.59	N
ATOM	1981	CA	ILE	A	256	15.740	-19.140	23.482	1.00	53.88	C
ATOM	1982	C	ILE	A	256	14.863	-20.362	23.227	1.00	55.73	C
ATOM	1983	O	ILE	A	256	14.031	-20.740	24.050	1.00	53.74	O
ATOM	1984	CB	ILE	A	256	16.721	-19.325	24.635	1.00	60.39	C
ATOM	1985	CG1	ILE	A	256	17.478	-18.003	24.865	1.00	49.75	C
ATOM	1986	CG2	ILE	A	256	17.729	-20.408	24.263	1.00	67.76	C
ATOM	1987	CD1	ILE	A	256	18.337	-17.959	26.113	1.00	52.15	C
ATOM	1988	N	ARG	A	257	15.049	-20.980	22.070	1.00	60.13	N
ATOM	1989	CA	ARG	A	257	14.153	-22.051	21.657	1.00	71.50	C
ATOM	1990	C	ARG	A	257	14.176	-23.516	22.065	1.00	69.32	C
ATOM	1991	O	ARG	A	257	13.160	-24.049	22.523	1.00	80.18	O
ATOM	1992	CB	ARG	A	257	14.007	-21.955	20.148	1.00	74.93	C
ATOM	1993	CG	ARG	A	257	13.281	-20.678	19.720	1.00	86.48	C
ATOM	1994	CD	ARG	A	257	11.972	-21.046	19.067	1.00	94.98	C
ATOM	1995	NE	ARG	A	257	12.243	-22.177	18.190	1.00	102.55	N
ATOM	1996	CZ	ARG	A	257	11.403	-23.175	17.936	1.00	101.10	C
ATOM	1997	NH1	ARG	A	257	10.194	-23.198	18.481	1.00	98.39	N
ATOM	1998	NH2	ARG	A	257	11.805	-24.190	17.182	1.00	99.09	N
ATOM	1999	N	ASN	A	258	15.287	-24.195	21.864	1.00	61.69	N
ATOM	2000	CA	ASN	A	258	15.340	-25.602	22.253	1.00	64.49	C
ATOM	2001	C	ASN	A	258	16.465	-25.618	23.247	1.00	62.07	C
ATOM	2002	O	ASN	A	258	17.624	-25.892	22.925	1.00	55.85	O
ATOM	2003	CB	ASN	A	258	15.636	-26.481	21.041	1.00	66.15	C
ATOM	2004	CG	ASN	A	258	14.404	-26.716	20.191	1.00	68.75	C
ATOM	2005	OD1	ASN	A	258	13.379	-27.234	20.673	1.00	64.25	O
ATOM	2006	ND2	ASN	A	258	14.484	-26.329	18.926	1.00	70.00	N
ATOM	2007	N	VAL	A	259	16.094	-25.272	24.468	1.00	62.90	N
ATOM	2008	CA	VAL	A	259	17.049	-25.157	25.545	1.00	65.80	C
ATOM	2009	C	VAL	A	259	17.876	-26.384	25.872	1.00	58.88	C
ATOM	2010	O	VAL	A	259	17.365	-27.483	26.054	1.00	56.71	O
ATOM	2011	CB	VAL	A	259	16.370	-24.703	26.858	1.00	64.49	C
ATOM	2012	CG1	VAL	A	259	17.433	-24.328	27.883	1.00	63.04	C
ATOM	2013	CG2	VAL	A	259	15.437	-23.546	26.599	1.00	62.50	C
ATOM	2014	N	ASP	A	260	19.176	-26.159	25.951	1.00	60.37	N
ATOM	2015	CA	ASP	A	260	20.110	-27.191	26.329	1.00	64.76	C
ATOM	2016	C	ASP	A	260	21.141	-26.491	27.190	1.00	63.70	C
ATOM	2017	O	ASP	A	260	21.185	-25.257	27.253	1.00	55.60	O
ATOM	2018	CB	ASP	A	260	20.785	-27.829	25.120	1.00	61.25	C
ATOM	2019	CG	ASP	A	260	21.602	-26.844	24.322	1.00	68.49	C
ATOM	2020	OD1	ASP	A	260	22.091	-25.847	24.896	1.00	68.44	O
ATOM	2021	OD2	ASP	A	260	21.775	-27.084	23.110	1.00	81.31	O
ATOM	2022	N	LYS	A	261	21.986	-27.277	27.832	1.00	57.12	N
ATOM	2023	CA	LYS	A	261	22.985	-26.711	28.711	1.00	51.64	C
ATOM	2024	C	LYS	A	261	23.832	-25.591	28.141	1.00	46.97	C
ATOM	2025	O	LYS	A	261	24.335	-24.757	28.895	1.00	48.66	O

Figure 2 (Table 2 (page 44))

ATOM	2026	CB	LYS	A	261	23.874	-27.828	29.258	1.00	52.71	C
ATOM	2027	CG	LYS	A	261	23.193	-28.612	30.358	1.00	61.87	C
ATOM	2028	CD	LYS	A	261	24.105	-29.669	30.947	1.00	73.37	C
ATOM	2029	CE	LYS	A	261	23.600	-30.117	32.308	1.00	76.85	C
ATOM	2030	NZ	LYS	A	261	23.680	-29.007	33.304	1.00	77.99	N
ATOM	2031	N	ASN	A	262	24.004	-25.534	26.827	1.00	51.62	N
ATOM	2032	CA	ASN	A	262	24.834	-24.464	26.278	1.00	50.71	C
ATOM	2033	C	ASN	A	262	24.189	-23.099	26.414	1.00	49.52	C
ATOM	2034	O	ASN	A	262	24.835	-22.073	26.224	1.00	44.29	O
ATOM	2035	CB	ASN	A	262	25.160	-24.707	24.815	1.00	63.69	C
ATOM	2036	CG	ASN	A	262	26.545	-25.256	24.636	1.00	76.99	C
ATOM	2037	OD1	ASN	A	262	27.466	-24.881	25.368	1.00	88.03	O
ATOM	2038	ND2	ASN	A	262	26.713	-26.145	23.664	1.00	83.71	N
ATOM	2039	N	ASP	A	263	22.911	-23.100	26.755	1.00	43.87	N
ATOM	2040	CA	ASP	A	263	22.173	-21.864	26.915	1.00	49.29	C
ATOM	2041	C	ASP	A	263	22.341	-21.257	28.307	1.00	56.55	C
ATOM	2042	O	ASP	A	263	21.984	-20.103	28.532	1.00	45.77	O
ATOM	2043	CB	ASP	A	263	20.705	-22.115	26.593	1.00	46.15	C
ATOM	2044	CG	ASP	A	263	20.502	-22.558	25.148	1.00	47.16	C
ATOM	2045	OD1	ASP	A	263	21.208	-22.006	24.272	1.00	50.06	O
ATOM	2046	OD2	ASP	A	263	19.642	-23.440	24.894	1.00	53.96	O
ATOM	2047	N	GLU	A	264	22.886	-22.033	29.241	1.00	52.20	N
ATOM	2048	CA	GLU	A	264	23.126	-21.517	30.580	1.00	50.47	C
ATOM	2049	C	GLU	A	264	24.217	-20.455	30.464	1.00	55.25	C
ATOM	2050	O	GLU	A	264	25.286	-20.722	29.917	1.00	51.52	O
ATOM	2051	CB	GLU	A	264	23.575	-22.644	31.526	1.00	49.18	C
ATOM	2052	CG	GLU	A	264	23.865	-22.150	32.948	1.00	56.13	C
ATOM	2053	CD	GLU	A	264	24.070	-23.270	33.968	1.00	59.96	C
ATOM	2054	OE1	GLU	A	264	23.144	-24.088	34.166	1.00	52.27	O
ATOM	2055	OE2	GLU	A	264	25.161	-23.319	34.575	1.00	63.96	O
ATOM	2056	N	ALA	A	265	23.936	-19.254	30.971	1.00	50.58	N
ATOM	2057	CA	ALA	A	265	24.882	-18.143	30.932	1.00	49.56	C
ATOM	2058	C	ALA	A	265	24.285	-16.892	31.553	1.00	44.28	C
ATOM	2059	O	ALA	A	265	23.138	-16.876	32.020	1.00	44.60	O
ATOM	2060	CB	ALA	A	265	25.275	-17.839	29.485	1.00	55.17	C
ATOM	2061	N	GLU	A	266	25.084	-15.837	31.565	1.00	46.95	N
ATOM	2062	CA	GLU	A	266	24.597	-14.566	32.052	1.00	58.95	C
ATOM	2063	C	GLU	A	266	24.233	-13.782	30.796	1.00	54.06	C
ATOM	2064	O	GLU	A	266	25.077	-13.547	29.937	1.00	49.16	O
ATOM	2065	CB	GLU	A	266	25.662	-13.784	32.824	1.00	49.59	C
ATOM	2066	CG	GLU	A	266	25.188	-12.371	33.185	1.00	68.76	C
ATOM	2067	CD	GLU	A	266	26.312	-11.461	33.655	1.00	79.04	C
ATOM	2068	OE1	GLU	A	266	27.442	-11.585	33.135	1.00	92.30	O
ATOM	2069	OE2	GLU	A	266	26.071	-10.604	34.534	1.00	84.00	O
ATOM	2070	N	TYR	A	267	22.969	-13.405	30.682	1.00	56.50	N
ATOM	2071	CA	TYR	A	267	22.539	-12.620	29.539	1.00	53.55	C
ATOM	2072	C	TYR	A	267	22.379	-11.175	29.973	1.00	53.33	C
ATOM	2073	O	TYR	A	267	21.857	-10.899	31.051	1.00	56.26	O
ATOM	2074	CB	TYR	A	267	21.216	-13.131	29.000	1.00	41.05	C
ATOM	2075	CG	TYR	A	267	21.302	-14.503	28.392	1.00	52.19	C
ATOM	2076	CD1	TYR	A	267	21.310	-15.645	29.200	1.00	46.18	C
ATOM	2077	CD2	TYR	A	267	21.374	-14.669	27.010	1.00	42.85	C
ATOM	2078	CE1	TYR	A	267	21.385	-16.907	28.649	1.00	36.41	C
ATOM	2079	CE2	TYR	A	267	21.447	-15.926	26.447	1.00	47.87	C
ATOM	2080	CZ	TYR	A	267	21.454	-17.043	27.269	1.00	46.20	C
ATOM	2081	OH	TYR	A	267	21.534	-18.289	26.709	1.00	46.42	O

Figure 2 (Table 2 (page 45))

ATOM	2082	N	VAL	A	268	22.849	-10.259	29.134	1.00	54.55	N
ATOM	2083	CA	VAL	A	268	22.744	-8.833	29.420	1.00	51.27	C
ATOM	2084	C	VAL	A	268	21.939	-8.121	28.325	1.00	53.04	C
ATOM	2085	O	VAL	A	268	22.238	-8.268	27.140	1.00	49.32	O
ATOM	2086	CB	VAL	A	268	24.149	-8.164	29.507	1.00	51.72	C
ATOM	2087	CG1	VAL	A	268	24.008	-6.653	29.697	1.00	53.25	C
ATOM	2088	CG2	VAL	A	268	24.954	-8.757	30.667	1.00	53.72	C
ATOM	2089	N	CYS	A	269	20.909	-7.372	28.708	1.00	47.02	N
ATOM	2090	CA	CYS	A	269	20.130	-6.631	27.712	1.00	46.07	C
ATOM	2091	C	CYS	A	269	20.572	-5.192	27.825	1.00	48.28	C
ATOM	2092	O	CYS	A	269	20.513	-4.568	28.893	1.00	54.75	O
ATOM	2093	CB	CYS	A	269	18.645	-6.725	27.972	1.00	47.89	C
ATOM	2094	SG	CYS	A	269	18.154	-6.060	29.588	1.00	57.20	S
ATOM	2095	N	ILE	A	270	21.040	-4.684	26.705	1.00	44.49	N
ATOM	2096	CA	ILE	A	270	21.542	-3.334	26.618	1.00	54.21	C
ATOM	2097	C	ILE	A	270	20.492	-2.429	25.984	1.00	51.98	C
ATOM	2098	O	ILE	A	270	20.057	-2.665	24.858	1.00	52.39	O
ATOM	2099	CB	ILE	A	270	22.804	-3.333	25.757	1.00	58.16	C
ATOM	2100	CG1	ILE	A	270	23.777	-4.385	26.287	1.00	59.14	C
ATOM	2101	CG2	ILE	A	270	23.451	-1.964	25.768	1.00	58.07	C
ATOM	2102	CD1	ILE	A	270	24.907	-4.698	25.332	1.00	62.65	C
ATOM	2103	N	ALA	A	271	20.068	-1.413	26.725	1.00	46.08	N
ATOM	2104	CA	ALA	A	271	19.081	-0.463	26.220	1.00	43.82	C
ATOM	2105	C	ALA	A	271	19.811	0.838	25.863	1.00	41.91	C
ATOM	2106	O	ALA	A	271	20.461	1.454	26.713	1.00	41.51	O
ATOM	2107	CB	ALA	A	271	18.010	-0.212	27.272	1.00	40.50	C
ATOM	2108	N	GLU	A	272	19.709	1.242	24.601	1.00	43.98	N
ATOM	2109	CA	GLU	A	272	20.375	2.453	24.128	1.00	50.40	C
ATOM	2110	C	GLU	A	272	19.526	3.346	23.255	1.00	40.39	C
ATOM	2111	O	GLU	A	272	18.635	2.880	22.548	1.00	43.66	O
ATOM	2112	CB	GLU	A	272	21.589	2.115	23.251	1.00	46.89	C
ATOM	2113	CG	GLU	A	272	22.738	1.366	23.863	1.00	76.32	C
ATOM	2114	CD	GLU	A	272	23.835	1.101	22.832	1.00	88.35	C
ATOM	2115	OE1	GLU	A	272	23.496	0.886	21.643	1.00	95.66	O
ATOM	2116	OE2	GLU	A	272	25.031	1.096	23.206	1.00	91.47	O
ATOM	2117	N	ASN	A	273	19.843	4.635	23.316	1.00	46.76	N
ATOM	2118	CA	ASN	A	273	19.260	5.648	22.438	1.00	47.59	C
ATOM	2119	C	ASN	A	273	20.335	6.718	22.340	1.00	52.11	C
ATOM	2120	O	ASN	A	273	21.366	6.622	23.008	1.00	44.76	O
ATOM	2121	CB	ASN	A	273	17.897	6.201	22.916	1.00	46.27	C
ATOM	2122	CG	ASN	A	273	17.964	6.980	24.211	1.00	44.51	C
ATOM	2123	OD1	ASN	A	273	19.012	7.471	24.611	1.00	44.37	O
ATOM	2124	ND2	ASN	A	273	16.808	7.126	24.866	1.00	38.00	N
ATOM	2125	N	LYS	A	274	20.128	7.723	21.504	1.00	56.80	N
ATOM	2126	CA	LYS	A	274	21.154	8.740	21.317	1.00	51.83	C
ATOM	2127	C	LYS	A	274	21.618	9.485	22.567	1.00	54.11	C
ATOM	2128	O	LYS	A	274	22.667	10.123	22.545	1.00	58.51	O
ATOM	2129	CB	LYS	A	274	20.718	9.742	20.238	1.00	55.02	C
ATOM	2130	CG	LYS	A	274	19.590	10.658	20.644	1.00	47.96	C
ATOM	2131	CD	LYS	A	274	18.892	11.218	19.403	1.00	52.54	C
ATOM	2132	CE	LYS	A	274	19.784	12.175	18.622	1.00	65.50	C
ATOM	2133	NZ	LYS	A	274	19.120	12.652	17.364	1.00	68.41	N
ATOM	2134	N	ALA	A	275	20.869	9.403	23.659	1.00	47.65	N
ATOM	2135	CA	ALA	A	275	21.275	10.100	24.868	1.00	48.41	C
ATOM	2136	C	ALA	A	275	21.944	9.233	25.930	1.00	49.48	C
ATOM	2137	O	ALA	A	275	22.294	9.735	26.988	1.00	50.34	O

Figure 2 (Table 2 (page 46))

ATOM	2138	CB	ALA	A	275	20.084	10.814	25.487	1.00	44.55	C
ATOM	2139	N	GLY	A	276	22.122	7.942	25.691	1.00	49.34	N
ATOM	2140	CA	GLY	A	276	22.755	7.177	26.746	1.00	51.88	C
ATOM	2141	C	GLY	A	276	22.482	5.694	26.738	1.00	50.21	C
ATOM	2142	O	GLY	A	276	21.907	5.164	25.779	1.00	51.48	O
ATOM	2143	N	GLU	A	277	22.868	5.026	27.824	1.00	50.99	N
ATOM	2144	CA	GLU	A	277	22.696	3.586	27.906	1.00	53.05	C
ATOM	2145	C	GLU	A	277	22.598	3.056	29.316	1.00	51.11	C
ATOM	2146	O	GLU	A	277	23.116	3.655	30.249	1.00	52.32	O
ATOM	2147	CB	GLU	A	277	23.873	2.915	27.194	1.00	58.98	C
ATOM	2148	CG	GLU	A	277	23.900	1.389	27.218	1.00	74.31	C
ATOM	2149	CD	GLU	A	277	24.570	0.797	28.462	1.00	89.46	C
ATOM	2150	OE1	GLU	A	277	25.277	1.537	29.183	1.00	96.28	O
ATOM	2151	OE2	GLU	A	277	24.398	-0.420	28.705	1.00	89.19	O
ATOM	2152	N	GLN	A	278	21.907	1.927	29.453	1.00	49.66	N
ATOM	2153	CA	GLN	A	278	21.783	1.228	30.724	1.00	45.13	C
ATOM	2154	C	GLN	A	278	21.513	-0.239	30.415	1.00	50.42	C
ATOM	2155	O	GLN	A	278	20.877	-0.568	29.417	1.00	46.75	O
ATOM	2156	CB	GLN	A	278	20.662	1.789	31.607	1.00	48.09	C
ATOM	2157	CG	GLN	A	278	20.812	1.327	33.064	1.00	46.69	C
ATOM	2158	CD	GLN	A	278	19.700	1.822	33.976	1.00	57.97	C
ATOM	2159	OE1	GLN	A	278	18.572	1.330	33.917	1.00	44.46	O
ATOM	2160	NE2	GLN	A	278	20.012	2.800	34.826	1.00	53.33	N
ATOM	2161	N	ASP	A	279	22.013	-1.132	31.257	1.00	45.92	N
ATOM	2162	CA	ASP	A	279	21.795	-2.541	31.014	1.00	47.69	C
ATOM	2163	C	ASP	A	279	21.345	-3.251	32.270	1.00	47.71	C
ATOM	2164	O	ASP	A	279	21.357	-2.687	33.366	1.00	48.35	O
ATOM	2165	CB	ASP	A	279	23.062	-3.186	30.451	1.00	60.02	C
ATOM	2166	CG	ASP	A	279	24.316	-2.707	31.154	1.00	69.17	C
ATOM	2167	OD1	ASP	A	279	24.456	-2.954	32.370	1.00	75.17	O
ATOM	2168	OD2	ASP	A	279	25.157	-2.073	30.490	1.00	75.70	O
ATOM	2169	N	ALA	A	280	20.892	-4.480	32.079	1.00	49.27	N
ATOM	2170	CA	ALA	A	280	20.428	-5.314	33.172	1.00	57.28	C
ATOM	2171	C	ALA	A	280	20.804	-6.748	32.833	1.00	54.10	C
ATOM	2172	O	ALA	A	280	20.868	-7.126	31.659	1.00	47.63	O
ATOM	2173	CB	ALA	A	280	18.909	-5.184	33.341	1.00	47.77	C
ATOM	2174	N	SER	A	281	21.043	-7.560	33.854	1.00	53.68	N
ATOM	2175	CA	SER	A	281	21.429	-8.931	33.599	1.00	48.69	C
ATOM	2176	C	SER	A	281	20.402	-9.952	34.031	1.00	45.20	C
ATOM	2177	O	SER	A	281	19.595	-9.718	34.934	1.00	45.89	O
ATOM	2178	CB	SER	A	281	22.768	-9.219	34.279	1.00	61.38	C
ATOM	2179	OG	SER	A	281	22.718	-8.863	35.646	1.00	57.59	O
ATOM	2180	N	ILE	A	282	20.427	-11.086	33.349	1.00	43.38	N
ATOM	2181	CA	ILE	A	282	19.524	-12.185	33.637	1.00	41.38	C
ATOM	2182	C	ILE	A	282	20.392	-13.429	33.671	1.00	47.86	C
ATOM	2183	O	ILE	A	282	21.235	-13.631	32.799	1.00	51.03	O
ATOM	2184	CB	ILE	A	282	18.436	-12.316	32.548	1.00	40.14	C
ATOM	2185	CG1	ILE	A	282	17.557	-11.056	32.557	1.00	46.94	C
ATOM	2186	CG2	ILE	A	282	17.576	-13.549	32.807	1.00	42.53	C
ATOM	2187	CD1	ILE	A	282	16.484	-10.998	31.476	1.00	45.40	C
ATOM	2188	N	HIS	A	283	20.204	-14.248	34.695	1.00	45.39	N
ATOM	2189	CA	HIS	A	283	20.998	-15.458	34.816	1.00	46.01	C
ATOM	2190	C	HIS	A	283	20.145	-16.651	34.501	1.00	41.84	C
ATOM	2191	O	HIS	A	283	19.164	-16.923	35.197	1.00	51.27	O
ATOM	2192	CB	HIS	A	283	21.570	-15.575	36.230	1.00	53.96	C
ATOM	2193	CG	HIS	A	283	22.617	-14.551	36.543	1.00	60.28	C

Figure 2 (Table 2 (page 47))

ATOM	2194	ND1	HIS	A	283	23.908	-14.633	36.065	1.00	69.25	N
ATOM	2195	CD2	HIS	A	283	22.554	-13.401	37.260	1.00	68.71	C
ATOM	2196	CE1	HIS	A	283	24.593	-13.578	36.473	1.00	75.43	C
ATOM	2197	NE2	HIS	A	283	23.796	-12.816	37.199	1.00	66.88	N
ATOM	2198	N	LEU	A	284	20.499	-17.349	33.427	1.00	41.70	N
ATOM	2199	CA	LEU	A	284	19.752	-18.534	33.050	1.00	45.86	C
ATOM	2200	C	LEU	A	284	20.533	-19.778	33.469	1.00	49.53	C
ATOM	2201	O	LEU	A	284	21.683	-19.963	33.058	1.00	45.44	O
ATOM	2202	CB	LEU	A	284	19.515	-18.576	31.532	1.00	41.74	C
ATOM	2203	CG	LEU	A	284	18.782	-19.827	31.028	1.00	47.91	C
ATOM	2204	CD1	LEU	A	284	17.407	-19.888	31.680	1.00	45.59	C
ATOM	2205	CD2	LEU	A	284	18.648	-19.810	29.500	1.00	48.70	C
ATOM	2206	N	LYS	A	285	19.913	-20.625	34.285	1.00	48.59	N
ATOM	2207	CA	LYS	A	285	20.557	-21.863	34.711	1.00	53.60	C
ATOM	2208	C	LYS	A	285	19.797	-23.008	34.061	1.00	46.75	C
ATOM	2209	O	LYS	A	285	18.570	-23.061	34.109	1.00	49.33	O
ATOM	2210	CB	LYS	A	285	20.531	-21.991	36.239	1.00	56.58	C
ATOM	2211	CG	LYS	A	285	21.302	-20.880	36.942	1.00	63.01	C
ATOM	2212	CD	LYS	A	285	21.254	-21.021	38.459	1.00	71.05	C
ATOM	2213	CE	LYS	A	285	21.853	-19.795	39.148	1.00	76.77	C
ATOM	2214	NZ	LYS	A	285	20.993	-18.583	39.020	1.00	73.22	N
ATOM	2215	N	VAL	A	286	20.525	-23.922	33.436	1.00	44.47	N
ATOM	2216	CA	VAL	A	286	19.888	-25.047	32.759	1.00	53.73	C
ATOM	2217	C	VAL	A	286	20.271	-26.367	33.410	1.00	58.55	C
ATOM	2218	O	VAL	A	286	21.446	-26.709	33.489	1.00	58.02	O
ATOM	2219	CB	VAL	A	286	20.283	-25.078	31.268	1.00	49.11	C
ATOM	2220	CG1	VAL	A	286	19.618	-26.248	30.572	1.00	52.83	C
ATOM	2221	CG2	VAL	A	286	19.872	-23.760	30.597	1.00	49.45	C
ATOM	2222	N	PHE	A	287	19.267	-27.100	33.875	1.00	56.62	N
ATOM	2223	CA	PHE	A	287	19.493	-28.379	34.528	1.00	60.81	C
ATOM	2224	C	PHE	A	287	19.172	-29.540	33.607	1.00	64.78	C
ATOM	2225	O	PHE	A	287	18.208	-29.487	32.846	1.00	64.16	O
ATOM	2226	CB	PHE	A	287	18.645	-28.461	35.795	1.00	58.95	C
ATOM	2227	CG	PHE	A	287	18.868	-27.314	36.724	1.00	61.24	C
ATOM	2228	CD1	PHE	A	287	17.963	-26.259	36.783	1.00	56.19	C
ATOM	2229	CD2	PHE	A	287	20.036	-27.237	37.477	1.00	62.69	C
ATOM	2230	CE1	PHE	A	287	18.224	-25.139	37.575	1.00	53.03	C
ATOM	2231	CE2	PHE	A	287	20.304	-26.124	38.266	1.00	58.31	C
ATOM	2232	CZ	PHE	A	287	19.397	-25.073	38.314	1.00	59.07	C
ATOM	2233	N	ALA	A	288	19.997	-30.583	33.666	1.00	66.33	N
ATOM	2234	CA	ALA	A	288	19.795	-31.766	32.834	1.00	73.18	C
ATOM	2235	C	ALA	A	288	18.428	-32.377	33.119	1.00	78.08	C
ATOM	2236	O	ALA	A	288	17.960	-32.349	34.259	1.00	78.39	O
ATOM	2237	CB	ALA	A	288	20.887	-32.785	33.106	1.00	69.96	C
ATOM	2238	N	LYS	A	289	17.794	-32.931	32.087	1.00	80.55	N
ATOM	2239	CA	LYS	A	289	16.476	-33.541	32.240	1.00	84.08	C
ATOM	2240	C	LYS	A	289	16.535	-34.855	33.016	1.00	88.56	C
ATOM	2241	O	LYS	A	289	15.585	-35.127	33.785	1.00	92.60	O
ATOM	2242	CB	LYS	A	289	15.830	-33.779	30.872	1.00	82.11	C
ATOM	2243	CG	LYS	A	289	16.538	-34.804	30.009	1.00	82.83	C
ATOM	2244	CD	LYS	A	289	15.739	-35.066	28.748	1.00	81.13	C
ATOM	2245	CE	LYS	A	289	16.362	-36.164	27.910	1.00	87.98	C
ATOM	2246	NZ	LYS	A	289	15.562	-36.424	26.677	1.00	90.82	N
ATOM	2247	OXT	LYS	A	289	17.519	-35.608	32.835	1.00	94.14	O
TER	2248		LYS	A	289						
HETATM	2249	O	HOH		1	26.862	53.829	-2.499	1.00	53.80	O



Figure 2 (Table 2 (page 48))

HETATM	2250	O	HOH	2	31.435	56.206	-5.661	1.00	53.53	O
HETATM	2251	O	HOH	4	18.815	60.633	-12.908	1.00	43.98	O
HETATM	2252	O	HOH	5	16.291	34.157	5.585	1.00	64.41	O
HETATM	2253	O	HOH	6	24.283	23.825	11.233	1.00	59.48	O
HETATM	2254	O	HOH	7	21.204	19.365	17.749	1.00	60.83	O
HETATM	2255	O	HOH	8	15.430	12.803	19.226	1.00	45.67	O
HETATM	2256	O	HOH	9	22.245	15.815	31.410	1.00	50.19	O
HETATM	2257	O	HOH	10	25.429	21.325	30.709	1.00	49.37	O
HETATM	2258	O	HOH	11	23.048	36.010	15.248	1.00	51.13	O
HETATM	2259	O	HOH	12	29.692	33.165	19.866	1.00	37.03	O
HETATM	2260	O	HOH	13	9.169	23.139	31.247	1.00	61.40	O
HETATM	2261	O	HOH	14	17.022	56.166	8.038	1.00	75.27	O
HETATM	2262	O	HOH	15	8.769	40.002	7.174	1.00	48.91	O
HETATM	2263	O	HOH	16	10.231	43.238	7.473	1.00	47.42	O
HETATM	2264	O	HOH	17	15.641	26.081	5.720	1.00	78.13	O
HETATM	2265	O	HOH	18	20.551	14.627	22.658	1.00	46.05	O
HETATM	2266	O	HOH	19	11.221	-2.472	26.804	1.00	52.85	O
HETATM	2267	O	HOH	20	13.041	60.224	-4.320	1.00	64.49	O
HETATM	2268	O	HOH	21	14.835	48.897	-2.048	1.00	85.96	O
HETATM	2269	O	HOH	22	29.546	51.498	-21.147	1.00	47.61	O
HETATM	2270	O	HOH	23	24.511	42.141	-28.698	1.00	76.55	O
HETATM	2271	O	HOH	25	21.636	45.365	-18.499	1.00	37.40	O
HETATM	2272	O	HOH	26	15.790	47.805	-19.728	1.00	64.11	O
HETATM	2273	O	HOH	27	20.999	58.533	-6.980	1.00	47.49	O
HETATM	2274	O	HOH	28	14.534	40.436	5.659	1.00	59.32	O
HETATM	2275	O	HOH	29	18.746	16.322	14.473	1.00	79.28	O
HETATM	2276	O	HOH	30	25.965	40.212	9.533	1.00	52.16	O
HETATM	2277	O	HOH	31	16.482	55.396	13.144	1.00	59.76	O
HETATM	2278	O	HOH	32	9.922	15.732	20.883	1.00	48.37	O
HETATM	2279	O	HOH	33	11.915	-0.137	41.445	1.00	73.91	O
HETATM	2280	O	HOH	34	11.044	7.531	19.815	1.00	49.89	O
HETATM	2281	O	HOH	35	6.902	3.742	25.922	1.00	63.36	O
HETATM	2282	O	HOH	37	21.399	-1.338	20.994	1.00	76.17	O
HETATM	2283	O	HOH	38	18.329	53.773	-1.977	1.00	62.61	O
HETATM	2284	O	HOH	39	18.014	43.718	-2.937	1.00	49.73	O
HETATM	2285	O	HOH	40	32.281	40.568	-12.177	1.00	66.60	O
HETATM	2286	O	HOH	41	19.381	44.469	-19.805	1.00	64.16	O
HETATM	2287	O	HOH	42	25.046	41.566	-20.577	1.00	61.50	O
HETATM	2288	O	HOH	46	7.104	2.690	28.661	1.00	90.82	O
HETATM	2289	O	HOH	48	29.774	-14.171	32.170	1.00	72.60	O
HETATM	2290	O	HOH	49	36.677	48.530	-18.261	1.00	57.32	O
HETATM	2291	O	HOH	50	33.317	46.204	-17.946	1.00	47.09	O
HETATM	2292	O	HOH	52	22.357	37.802	16.682	1.00	62.95	O
HETATM	2293	O	HOH	54	11.598	9.583	18.307	1.00	51.71	O
HETATM	2294	O	HOH	55	22.448	12.959	33.086	1.00	71.24	O
HETATM	2295	O	HOH	56	12.323	-25.457	30.778	1.00	69.54	O
HETATM	2296	O	HOH	57	22.080	16.779	21.536	1.00	49.07	O
HETATM	2297	O	HOH	58	17.068	4.212	19.556	1.00	71.54	O
HETATM	2298	O	HOH	59	21.824	23.695	19.290	1.00	44.38	O
HETATM	2299	O	HOH	60	17.965	7.263	19.831	1.00	45.41	O
HETATM	2300	O	HOH	61	19.593	-1.710	35.113	1.00	49.69	O
HETATM	2301	O	HOH	62	18.642	-7.793	36.955	1.00	68.54	O
HETATM	2302	O	HOH	63	23.848	-0.227	33.498	1.00	54.90	O
HETATM	2303	O	HOH	64	31.052	-17.541	34.986	1.00	68.80	O
HETATM	2304	O	HOH	65	5.551	-4.238	9.968	1.00	64.86	O
HETATM	2305	O	HOH	66	10.472	-3.423	9.588	1.00	81.77	O

Figure 2 (Table 2 (page 49))

HETATM	2306	O	HOH	67	6.705	-3.198	12.269	1.00	59.36	O
HETATM	2307	O	HOH	68	18.934	8.523	16.255	1.00	70.67	O
HETATM	2308	O	HOH	69	26.373	-11.223	28.910	1.00	53.04	O
HETATM	2309	O	HOH	70	26.631	6.184	27.729	1.00	74.30	O
HETATM	2310	O	HOH	71	26.466	-20.918	34.876	1.00	70.68	O
HETATM	2311	O	HOH	72	8.293	12.647	18.395	1.00	56.61	O
HETATM	2312	O	HOH	74	17.106	-5.693	36.496	1.00	48.96	O
HETATM	2313	O	HOH	75	1.311	-8.583	8.383	1.00	70.05	O
HETATM	2314	O	HOH	76	26.233	40.015	4.081	1.00	64.69	O
HETATM	2315	O	HOH	77	21.018	39.423	0.780	1.00	63.73	O
HETATM	2316	O	HOH	78	30.385	47.077	-9.984	1.00	47.01	O
HETATM	2317	O	HOH	80	17.757	22.465	9.580	1.00	54.37	O
HETATM	2318	O	HOH	81	25.847	39.446	18.635	1.00	61.83	O
HETATM	2319	O	HOH	82	23.903	-18.248	35.163	1.00	66.46	O
HETATM	2320	O	HOH	83	17.550	29.059	7.625	1.00	69.50	O
HETATM	2321	O	HOH	84	22.192	30.581	38.779	1.00	45.18	O
HETATM	2322	O	HOH	85	19.724	26.758	8.865	1.00	62.11	O
HETATM	2323	O	HOH	87	29.601	58.691	-24.045	1.00	49.94	O
HETATM	2324	O	HOH	88	22.701	60.581	-7.832	1.00	65.08	O
HETATM	2325	O	HOH	89	21.940	62.739	-12.104	1.00	60.23	O
HETATM	2326	O	HOH	90	28.142	44.638	-19.542	1.00	52.86	O
HETATM	2327	O	HOH	91	19.926	59.567	-10.713	1.00	54.05	O
HETATM	2328	O	HOH	92	23.841	23.097	24.364	1.00	55.20	O
HETATM	2329	O	HOH	93	14.026	37.104	24.024	1.00	50.35	O
HETATM	2330	O	HOH	94	28.637	30.316	16.747	1.00	47.63	O
HETATM	2331	O	HOH	95	13.597	-12.079	32.292	1.00	47.38	O
HETATM	2332	O	HOH	96	20.525	6.030	31.726	1.00	59.12	O
HETATM	2333	O	HOH	97	12.219	25.294	38.142	1.00	74.46	O
HETATM	2334	O	HOH	98	17.582	46.166	-21.327	1.00	58.26	O
HETATM	2335	O	HOH	99	18.462	3.098	17.614	1.00	74.29	O
HETATM	2336	O	HOH	100	7.657	-6.217	21.068	1.00	54.31	O
HETATM	2337	O	HOH	101	31.973	58.468	-22.566	1.00	51.37	O
HETATM	2338	O	HOH	102	25.581	34.891	15.303	1.00	62.92	O
HETATM	2339	O	HOH	103	9.781	4.793	26.865	1.00	52.97	O
HETATM	2340	O	HOH	104	27.113	28.768	14.346	1.00	46.27	O
HETATM	2341	O	HOH	105	20.934	59.591	-4.081	1.00	63.10	O
HETATM	2342	O	HOH	106	29.101	39.039	-6.576	1.00	50.94	O
HETATM	2343	O	HOH	107	20.829	-6.266	36.888	1.00	67.77	O
HETATM	2344	O	HOH	108	14.801	-6.395	38.213	1.00	57.81	O
HETATM	2345	O	HOH	109	21.412	-19.178	24.173	1.00	57.65	O
HETATM	2346	O	HOH	110	29.742	32.206	15.564	1.00	51.50	O
HETATM	2347	O	HOH	111	27.197	38.482	-3.772	1.00	57.43	O
HETATM	2348	O	HOH	112	23.730	20.567	24.733	1.00	63.78	O
HETATM	2349	O	HOH	113	15.996	50.339	-4.519	1.00	68.59	O
HETATM	2350	O	HOH	114	10.665	-4.867	34.503	1.00	53.34	O
HETATM	2351	O	HOH	115	6.955	17.535	26.540	1.00	72.17	O
HETATM	2352	O	HOH	116	15.712	-29.078	24.014	1.00	65.77	O
HETATM	2353	O	HOH	118	32.255	44.366	-7.537	1.00	62.15	O
HETATM	2354	O	HOH	119	29.827	41.068	-0.664	1.00	57.67	O
HETATM	2355	O	HOH	122	14.630	-27.859	26.706	1.00	65.41	O
HETATM	2356	O	HOH	123	8.521	-18.764	25.803	1.00	74.48	O
HETATM	2357	O	HOH	125	15.199	60.049	-12.759	1.00	63.41	O
HETATM	2358	O	HOH	126	10.378	14.473	18.707	1.00	52.05	O
HETATM	2359	O	HOH	127	28.187	-10.553	30.862	1.00	65.81	O
HETATM	2360	O	HOH	128	7.837	37.705	8.662	1.00	62.54	O
HETATM	2361	O	HOH	130	23.744	37.155	1.565	1.00	65.13	O

Figure 2 (Table 2 (page 50))

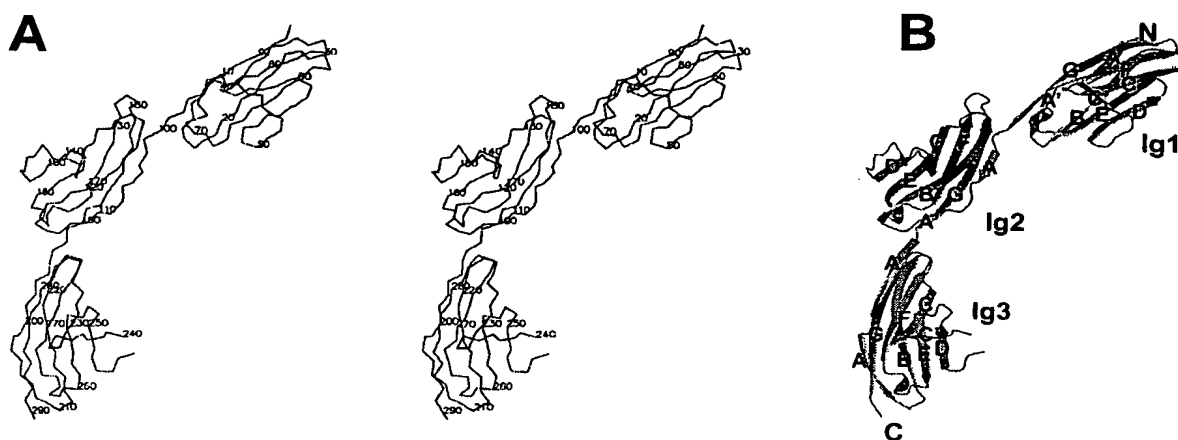
HETATM	2362	O	HOH	131	13.354	57.052	-9.380	1.00	64.16	O
HETATM	2363	O	HOH	132	31.235	44.417	-16.467	1.00	58.09	O
HETATM	2364	O	HOH	134	18.966	44.757	7.268	1.00	51.54	O
HETATM	2365	O	HOH	135	22.888	3.287	35.759	1.00	66.29	O
HETATM	2366	O	HOH	136	10.345	29.244	10.371	1.00	53.80	O
HETATM	2367	O	HOH	137	21.314	-8.331	20.298	1.00	59.91	O
HETATM	2368	O	HOH	138	38.747	55.169	-17.210	1.00	61.68	O
HETATM	2369	O	HOH	139	14.760	55.271	10.174	1.00	55.52	O
HETATM	2370	O	HOH	140	23.711	55.591	3.512	1.00	78.73	O
HETATM	2371	O	HOH	142	5.285	37.922	7.977	1.00	63.10	O
HETATM	2372	O	HOH	143	24.355	15.578	30.186	1.00	68.63	O
HETATM	2373	O	HOH	144	23.201	9.987	31.463	1.00	64.84	O
HETATM	2374	O	HOH	145	15.111	-8.434	40.304	1.00	70.85	O
HETATM	2375	O	HOH	146	34.105	49.705	-9.362	1.00	66.43	O
HETATM	2376	O	HOH	147	22.545	50.730	2.853	1.00	70.28	O
HETATM	2377	O	HOH	149	23.888	38.804	-17.868	1.00	69.84	O
HETATM	2378	O	HOH	150	26.301	66.907	-32.270	1.00	69.82	O
HETATM	2379	O	HOH	151	29.578	51.924	-24.078	1.00	67.26	O
HETATM	2380	O	HOH	152	31.935	49.759	-6.982	1.00	72.11	O
HETATM	2381	O	HOH	153	11.771	12.964	31.927	1.00	70.57	O
HETATM	2382	O	HOH	154	14.696	6.619	31.148	1.00	64.86	O
HETATM	2383	O	HOH	155	33.398	69.714	-31.980	1.00	74.81	O
HETATM	2384	O	HOH	156	26.480	50.982	0.230	1.00	59.10	O
HETATM	2385	O	HOH	157	22.798	7.195	30.848	1.00	68.26	O
HETATM	2386	O	HOH	158	19.477	-6.906	18.703	1.00	72.82	O
HETATM	2387	O	HOH	159	13.208	60.522	-15.082	1.00	57.68	O
HETATM	2388	O	HOH	160	34.799	47.949	-14.048	1.00	71.55	O
HETATM	2389	O	HOH	161	12.156	-20.278	36.293	1.00	63.41	O
HETATM	2390	O	HOH	162	12.064	0.618	21.733	1.00	59.67	O
HETATM	2391	O	HOH	163	13.025	12.470	18.298	1.00	57.94	O
HETATM	2392	O	HOH	164	11.241	-6.036	37.279	1.00	66.37	O
HETATM	2393	O	HOH	165	15.326	30.761	7.083	1.00	72.54	O
HETATM	2394	O	HOH	166	24.166	26.288	8.146	1.00	80.46	O
HETATM	2395	O	HOH	167	18.532	37.307	28.877	1.00	52.52	O
HETATM	2396	O	HOH	169	19.929	10.591	15.027	1.00	79.89	O
HETATM	2397	O	HOH	171	18.161	19.995	12.208	1.00	88.12	O
HETATM	2398	O	HOH	172	25.181	-23.987	37.247	1.00	83.59	O
HETATM	2399	O	HOH	174	18.136	-3.696	37.260	1.00	58.69	O
HETATM	2400	O	HOH	175	9.790	35.898	8.924	1.00	68.04	O
HETATM	2401	O	HOH	176	39.649	55.783	-13.588	1.00	75.74	O
HETATM	2402	O	HOH	177	11.431	-13.326	32.112	1.00	68.92	O
HETATM	2403	O	HOH	178	15.462	13.080	15.436	1.00	72.04	O
HETATM	2404	O	HOH	179	10.845	-23.387	30.834	1.00	75.68	O
HETATM	2405	O	HOH	180	8.771	-8.704	37.430	1.00	69.36	O
HETATM	2406	O	HOH	181	21.236	41.306	-18.704	1.00	71.93	O
HETATM	2407	O	HOH	182	15.632	39.325	24.779	1.00	76.42	O
HETATM	2408	O	HOH	184	9.633	7.268	24.170	1.00	59.85	O
HETATM	2409	O	HOH	185	8.212	-4.659	26.095	1.00	73.13	O
HETATM	2410	O	HOH	187	22.544	-23.667	22.886	1.00	67.43	O
HETATM	2411	O	HOH	190	38.135	52.923	-18.866	1.00	60.86	O
HETATM	2412	O	HOH	192	13.987	-13.566	39.379	1.00	64.17	O
HETATM	2413	O	HOH	194	8.678	19.753	34.818	1.00	74.26	O
HETATM	2414	O	HOH	195	16.248	11.313	17.210	1.00	71.99	O
HETATM	2415	O	HOH	196	21.583	37.449	-18.466	1.00	74.25	O
HETATM	2416	O	HOH	197	18.608	13.183	13.886	1.00	69.55	O
HETATM	2417	O	HOH	199	32.100	47.030	-11.918	1.00	55.13	O

Figure 2 (Table 2 (page 51))

HETATM	2418	O	HOH	200	8.309	-2.904	23.865	1.00	78.50	O
HETATM	2419	O	HOH	201	27.690	42.102	3.955	1.00	77.78	O
HETATM	2420	O	HOH	204	13.069	56.872	-6.846	1.00	79.77	O
HETATM	2421	O	HOH	205	13.299	3.871	18.787	1.00	66.67	O
HETATM	2422	O	HOH	206	29.245	60.023	-30.224	1.00	60.72	O
HETATM	2423	O	HOH	208	14.879	-4.423	17.190	1.00	90.36	O
HETATM	2424	O	HOH	209	10.483	17.298	32.627	1.00	73.09	O
HETATM	2425	O	HOH	210	11.855	61.308	-30.434	1.00	88.84	O
HETATM	2426	O	HOH	211	13.217	40.439	25.017	1.00	85.86	O
HETATM	2427	O	HOH	213	7.822	-16.528	22.942	1.00	78.51	O
HETATM	2428	O	HOH	214	23.675	20.955	33.560	1.00	73.68	O
HETATM	2429	O	HOH	215	8.958	-13.070	31.871	1.00	66.49	O
HETATM	2430	O	HOH	216	13.965	9.052	16.630	1.00	67.53	O
HETATM	2431	O	HOH	220	8.596	-0.069	28.112	1.00	61.80	O
HETATM	2432	O	HOH	221	31.299	38.557	-18.341	1.00	61.93	O
HETATM	2433	O	HOH	222	20.516	15.336	17.249	1.00	62.41	O
HETATM	2434	O	HOH	223	32.487	45.347	-13.991	1.00	67.08	O
HETATM	2435	O	HOH	224	9.634	26.343	28.605	1.00	80.33	O
HETATM	2436	O	HOH	225	26.881	41.843	6.770	1.00	66.49	O
HETATM	2437	O	HOH	226	21.933	62.656	-9.449	1.00	77.20	O
HETATM	2438	O	HOH	227	16.939	-0.959	38.266	1.00	47.64	O
HETATM	2439	O	HOH	228	1.517	27.871	29.550	1.00	69.94	O
HETATM	2440	O	HOH	229	25.455	67.088	-17.467	1.00	70.28	O
HETATM	2441	O	HOH	231	22.761	36.354	-14.024	1.00	67.12	O
HETATM	2442	O	HOH	233	9.742	-18.263	29.864	1.00	71.11	O
HETATM	2443	O	HOH	236	9.749	-1.644	39.210	1.00	68.73	O
HETATM	2444	O	HOH	238	18.795	37.370	-0.374	1.00	70.06	O
HETATM	2445	O	HOH	239	28.893	-23.822	27.314	1.00	63.21	O
HETATM	2446	O	HOH	240	20.653	54.689	-2.794	1.00	69.17	O
HETATM	2447	O	HOH	241	32.703	57.255	-7.932	1.00	73.68	O
HETATM	2448	O	HOH	242	26.839	45.754	-28.862	1.00	73.66	O
HETATM	2449	O	HOH	243	21.145	36.229	-1.718	1.00	67.47	O
HETATM	2450	O	HOH	244	24.749	63.978	-31.459	1.00	70.06	O
HETATM	2451	O	HOH	245	15.031	42.223	-0.424	1.00	65.72	O
HETATM	2452	O	HOH	246	13.421	46.493	5.518	1.00	68.84	O
HETATM	2453	O	HOH	247	31.086	37.829	-20.633	1.00	67.16	O
HETATM	2454	O	HOH	249	16.331	24.733	8.656	1.00	80.75	O
HETATM	2455	O	HOH	250	34.686	48.482	-11.577	1.00	67.41	O
HETATM	2456	O	HOH	252	26.863	-21.667	27.711	1.00	73.87	O
HETATM	2457	O	HOH	253	25.486	24.675	5.799	1.00	94.36	O
HETATM	2458	O	HOH	255	19.570	-18.069	15.539	1.00	68.87	O
HETATM	2459	O	HOH	256	7.507	24.181	27.128	1.00	75.95	O
HETATM	2460	O	HOH	257	18.214	50.275	13.595	1.00	77.43	O
HETATM	2461	O	HOH	258	24.259	5.598	21.754	1.00	80.04	O
HETATM	2462	O	HOH	259	23.644	-9.401	38.458	1.00	73.87	O
HETATM	2463	O	HOH	260	29.288	57.908	-36.191	1.00	83.70	O
HETATM	2464	O	HOH	261	14.644	-13.020	15.667	1.00	67.62	O
HETATM	2465	O	HOH	262	16.016	47.827	16.745	1.00	77.21	O
HETATM	2466	O	HOH	263	19.538	-33.347	29.648	1.00	64.40	O
HETATM	2467	O	HOH	265	2.949	33.426	13.572	1.00	75.54	O
HETATM	2468	O	HOH	266	25.030	51.698	-23.955	1.00	72.53	O
HETATM	2469	O	HOH	267	29.126	34.667	-5.967	1.00	87.07	O
HETATM	2470	O	HOH	268	21.351	0.866	18.679	1.00	81.24	O
HETATM	2471	O	HOH	270	11.563	-28.282	33.256	1.00	88.99	O
HETATM	2472	O	HOH	273	25.953	36.560	-14.131	1.00	68.45	O
HETATM	2473	O	HOH	275	3.498	32.668	11.344	1.00	60.17	O

**Figure 2 (Table 2 (page 52))**

HETATM	2474	O	HOH	277		24.261	-20.185	20.738	1.00	69.47	O
HETATM	2475	O	HOH	279		16.935	12.111	32.241	1.00	61.50	O
HETATM	2476	O	HOH	281		6.985	31.018	33.495	1.00	82.04	O
HETATM	2477	O	HOH	282		29.259	66.155	-18.386	1.00	76.82	O
HETATM	2478	O	HOH	283		7.960	15.959	16.209	1.00	82.31	O
HETATM	2479	O	HOH	284		10.497	-27.436	17.219	1.00	87.04	O
HETATM	2480	O	HOH	286		26.964	63.396	-39.492	1.00	92.90	O
HETATM	2481	O	HOH	288		24.134	68.136	-30.170	1.00	73.68	O
HETATM	2482	O	HOH	289		21.035	57.596	-2.427	1.00	63.71	O
HETATM	2483	O	HOH	290		5.098	-6.663	9.498	1.00	71.30	O
HETATM	2484	O	HOH	291		28.355	60.022	-32.628	1.00	84.14	O
HETATM	2485	O	HOH	292		27.829	-18.993	32.106	1.00	83.61	O
HETATM	2486	O	HOH	294		25.765	53.781	-27.581	1.00	80.50	O
HETATM	2487	O	HOH	295		24.969	-15.013	17.181	1.00	79.45	O
HETATM	2488	O	HOH	296		21.804	-31.840	29.638	1.00	63.37	O
HETATM	2489	O	HOH	297		24.675	41.475	22.470	1.00	76.81	O
HETATM	2490	O	HOH	298		21.097	-16.469	16.858	1.00	76.40	O
HETATM	2491	O	HOH	299		10.492	1.947	39.785	1.00	73.55	O
HETATM	2492	O	HOH	300		24.883	60.577	-6.394	1.00	83.17	O
HETATM	2493	O	HOH	301		12.022	63.003	-25.379	1.00	82.86	O
HETATM	2494	O	HOH	302		29.658	36.500	-13.658	1.00	76.81	O
HETATM	2495	O	HOH	303		28.183	35.860	-10.762	1.00	71.74	O
HETATM	2496	O	HOH	304		33.215	39.854	-9.262	1.00	79.17	O
HETATM	2497	O	HOH	305		22.138	35.777	-10.127	1.00	75.26	O
HETATM	2498	O	HOH	306		34.862	51.476	-6.285	1.00	73.10	O
HETATM	2499	O	HOH	307		40.147	51.580	-7.567	1.00	79.78	O
HETATM	2500	O	HOH	308		28.423	71.917	-29.800	1.00	75.06	O
HETATM	2501	O	HOH	309		31.298	68.573	-22.781	1.00	78.92	O
HETATM	2502	O	HOH	310		22.252	33.788	4.586	1.00	75.58	O
HETATM	2503	O	HOH	311		26.312	13.773	26.214	1.00	71.75	O
HETATM	2504	O	HOH	312		24.723	12.029	25.114	1.00	75.67	O
HETATM	2505	O	HOH	313		23.485	49.266	5.646	1.00	72.55	O
HETATM	2506	O	HOH	314		25.648	43.055	12.920	1.00	71.36	O
HETATM	2507	O	HOH	315		4.653	34.503	32.710	1.00	77.71	O
HETATM	2508	O	HOH	316		2.456	37.131	32.175	1.00	78.77	O
HETATM	2509	O	HOH	317		6.881	27.100	34.488	1.00	80.24	O
HETATM	2510	O	HOH	318		10.082	23.711	13.099	1.00	81.07	O
HETATM	2511	O	HOH	319		18.524	-28.499	21.428	1.00	79.53	O
HETATM	2512	O	HOH	321		26.684	3.017	30.716	1.00	82.34	O
HETATM	2513	O	HOH	322		27.178	-5.228	32.903	1.00	8	

**Figure 3**

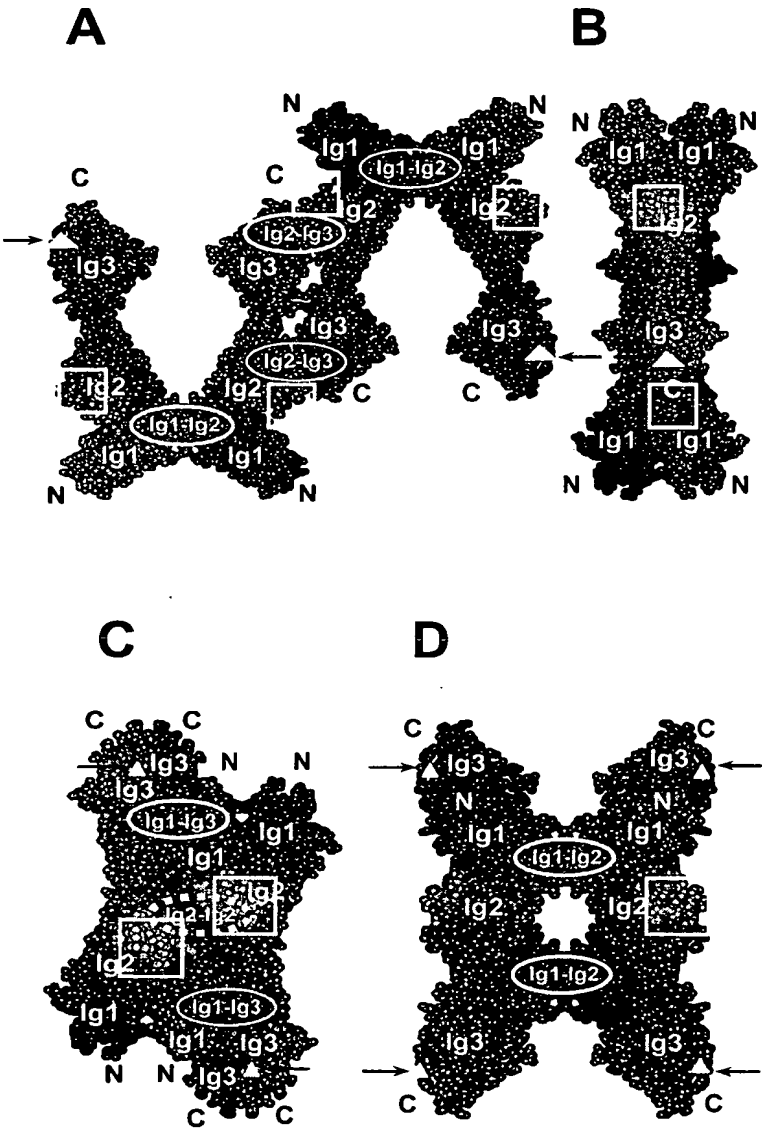


Figure 4

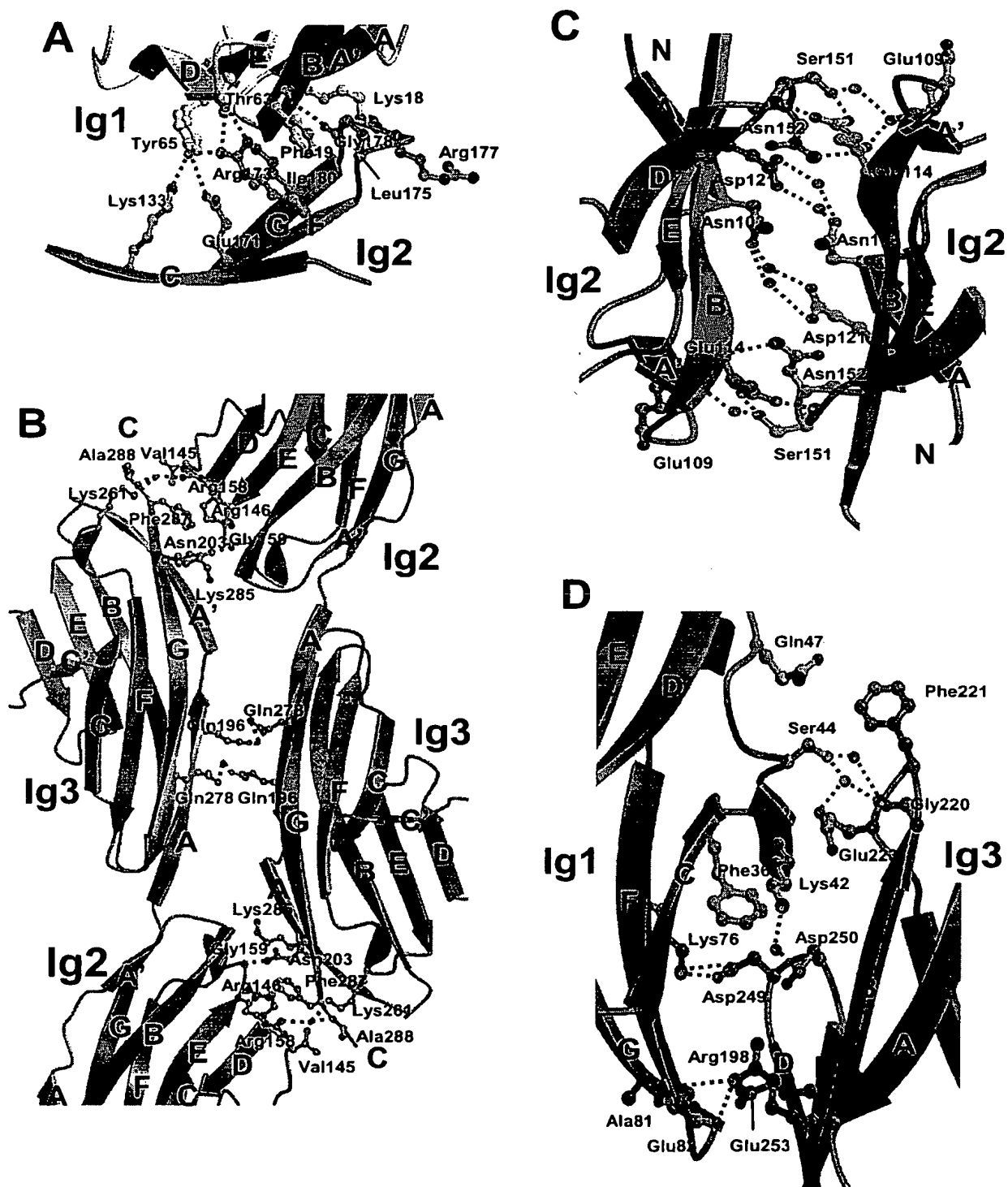


Figure 5



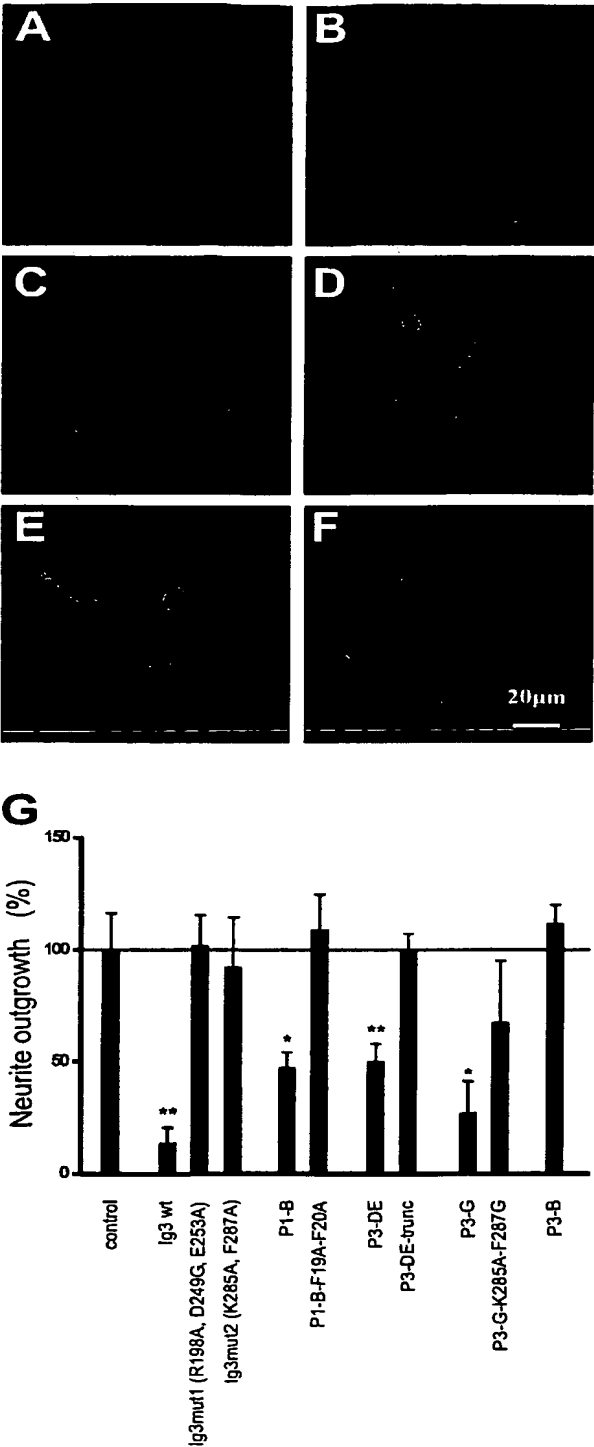
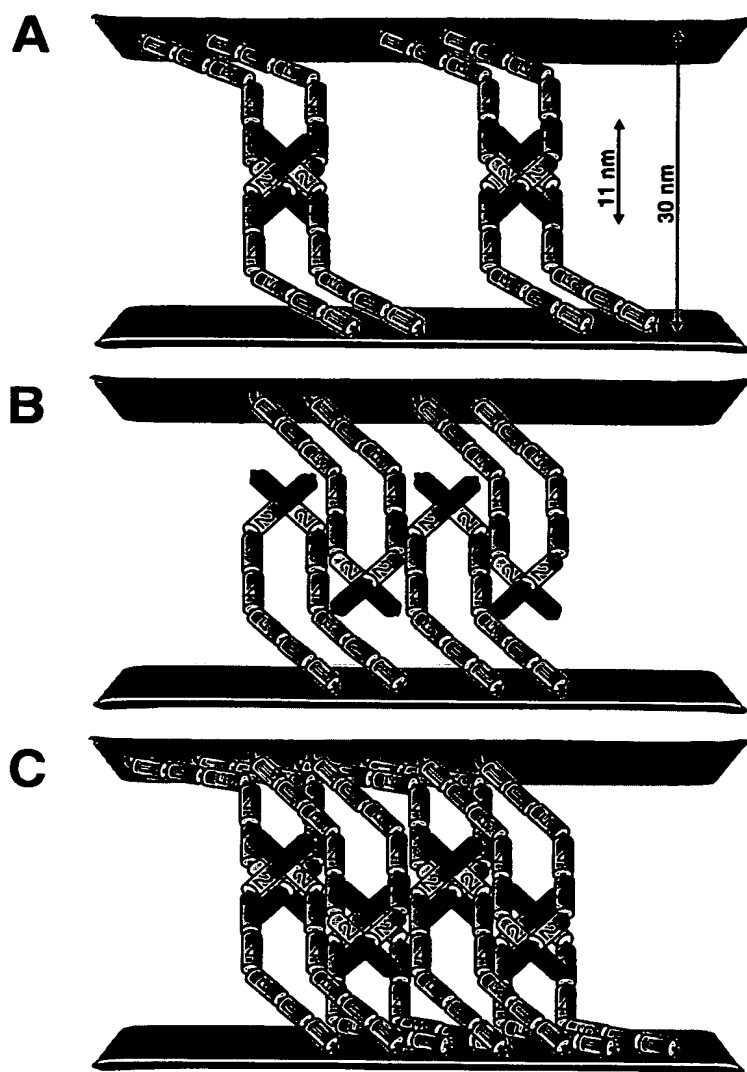
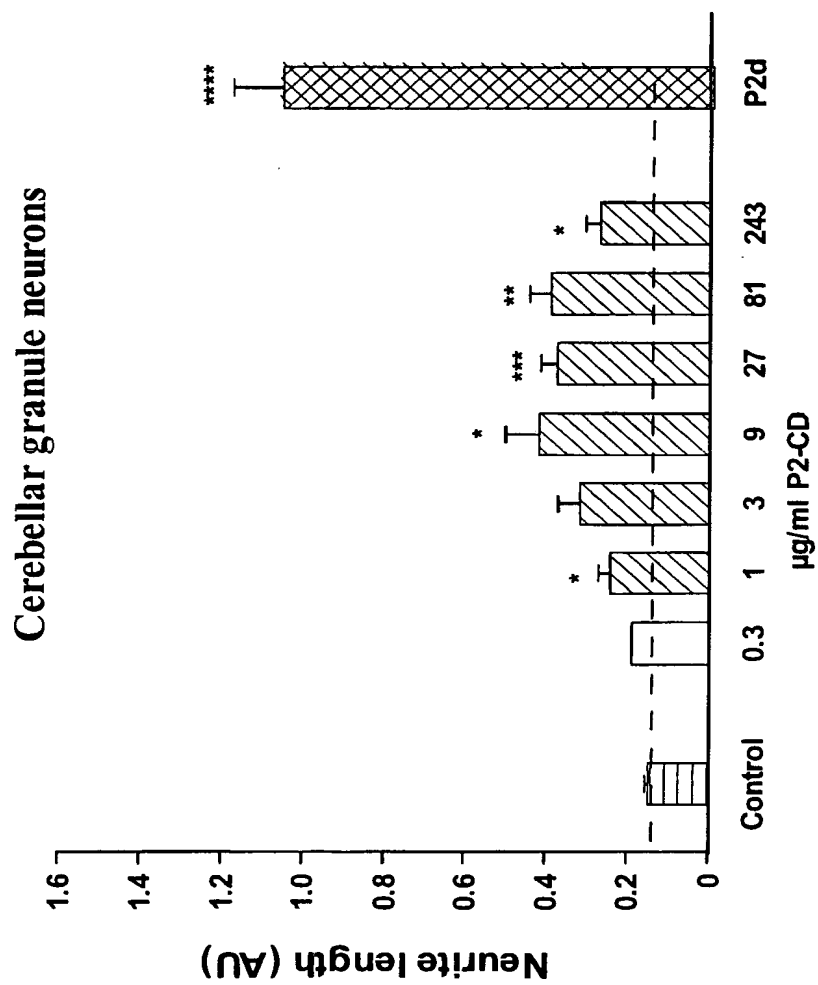


Figure 6

**Figure 7**

**Figure 8**

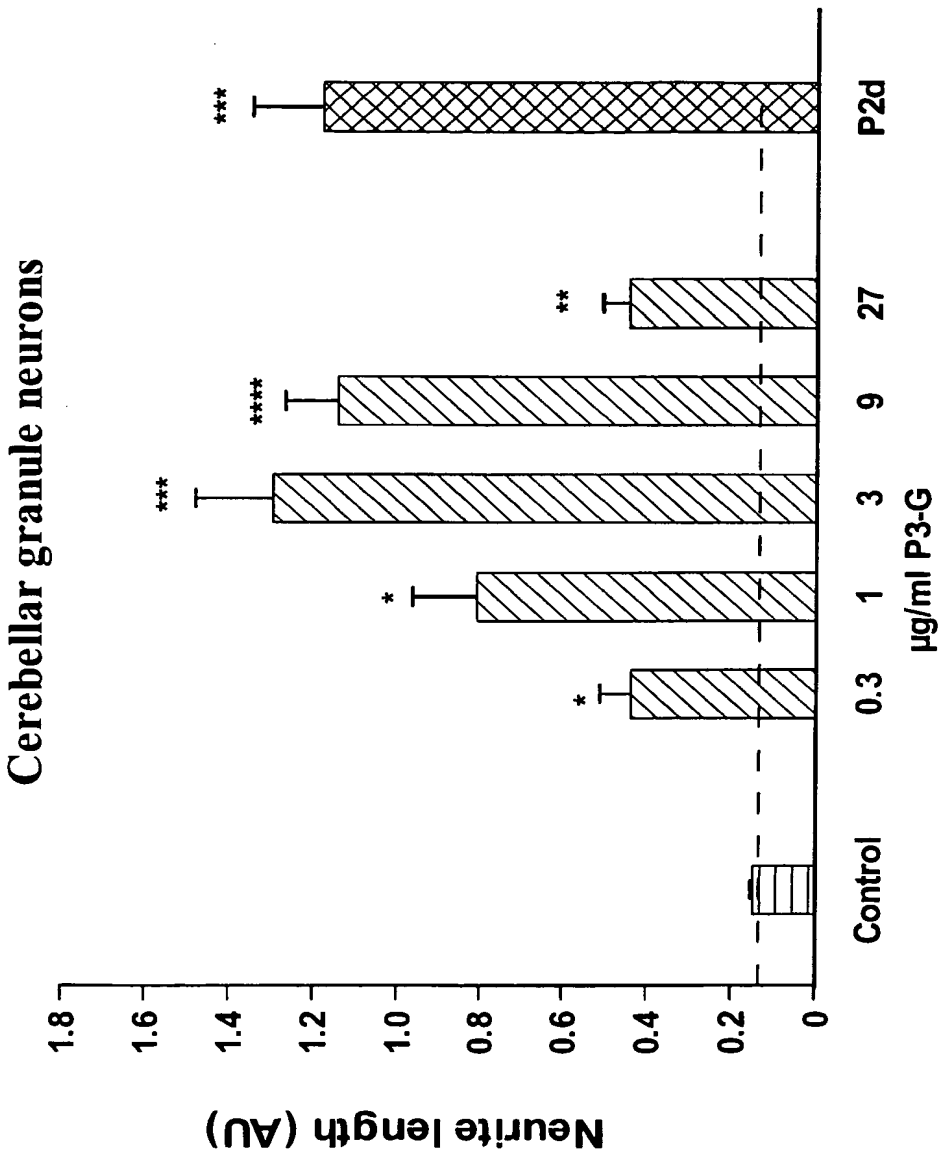


Figure 9

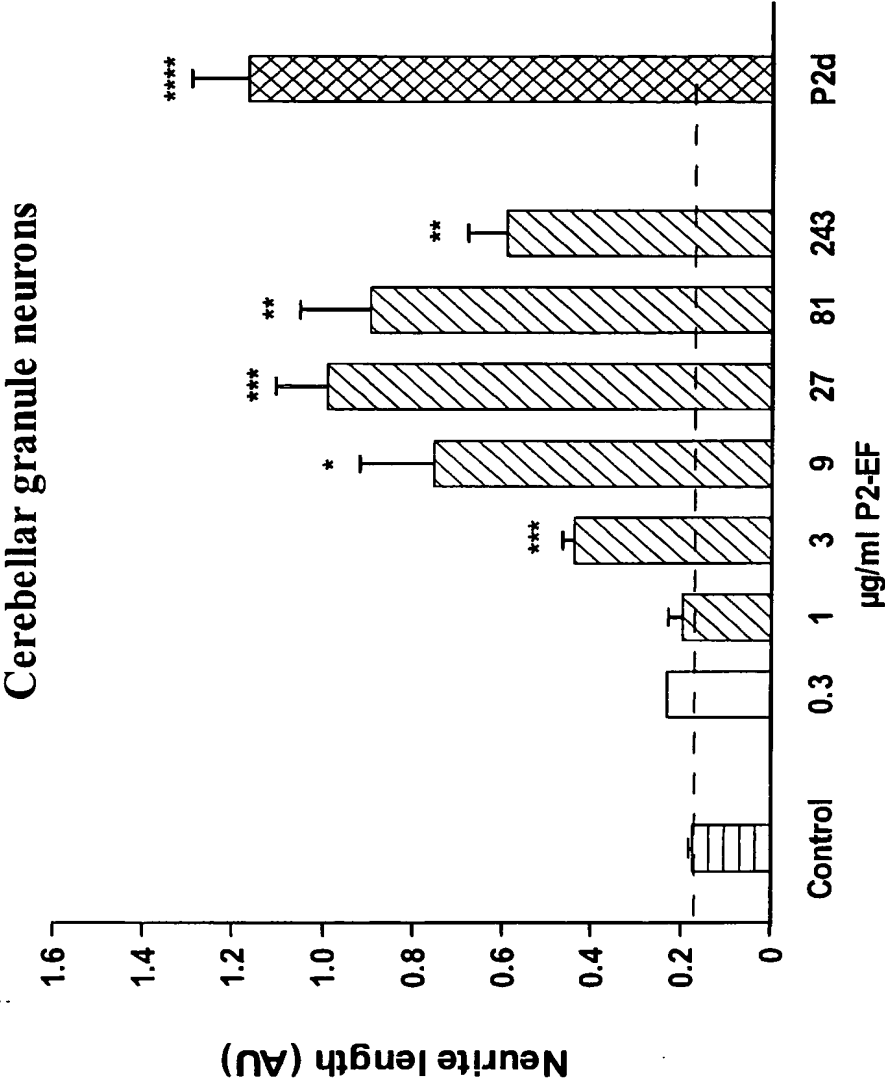
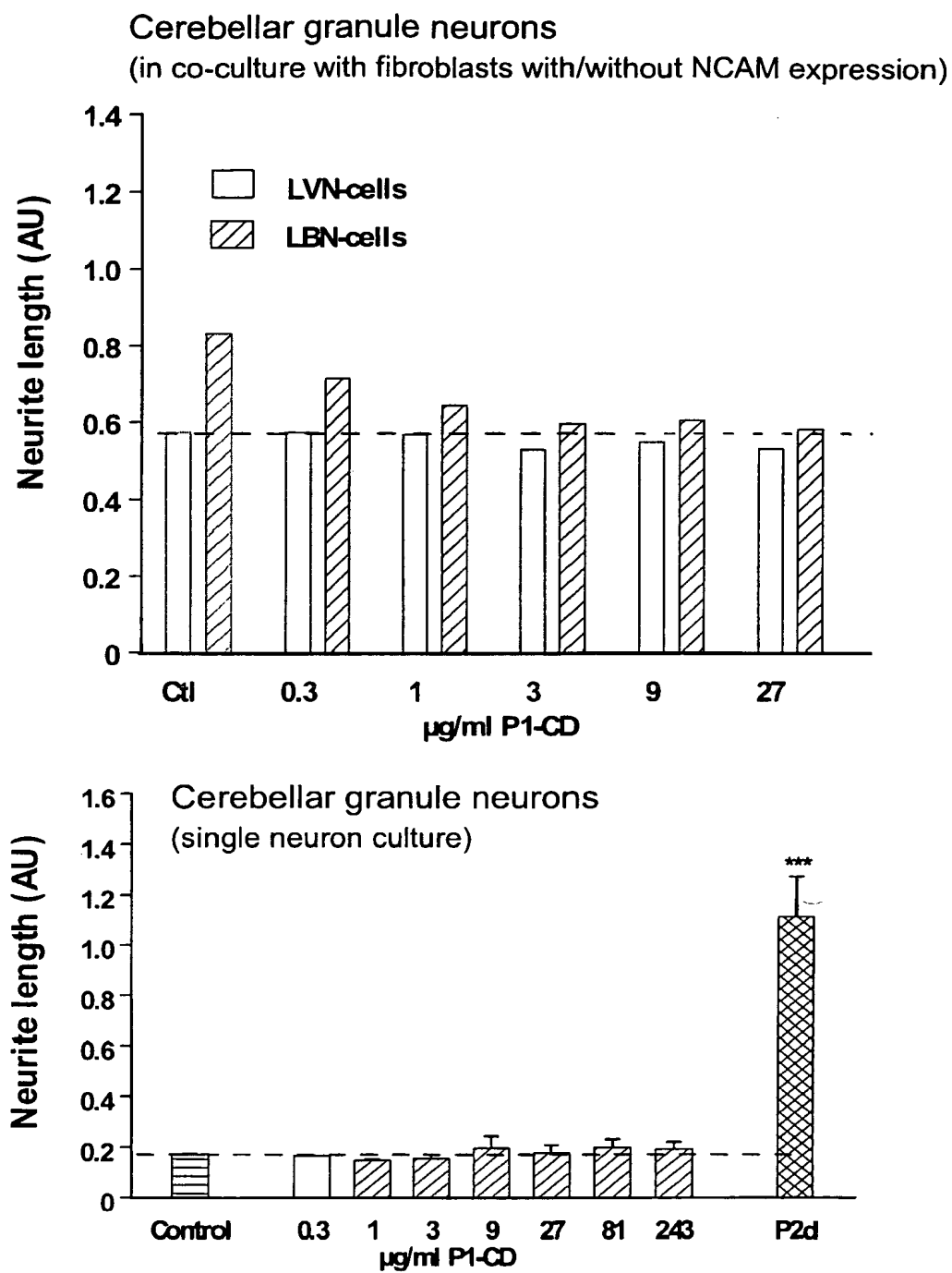


Figure 10

**Figure 11**

Cerebellar granule neurons  
(in co-culture with fibroblasts with/without NCAM expression)

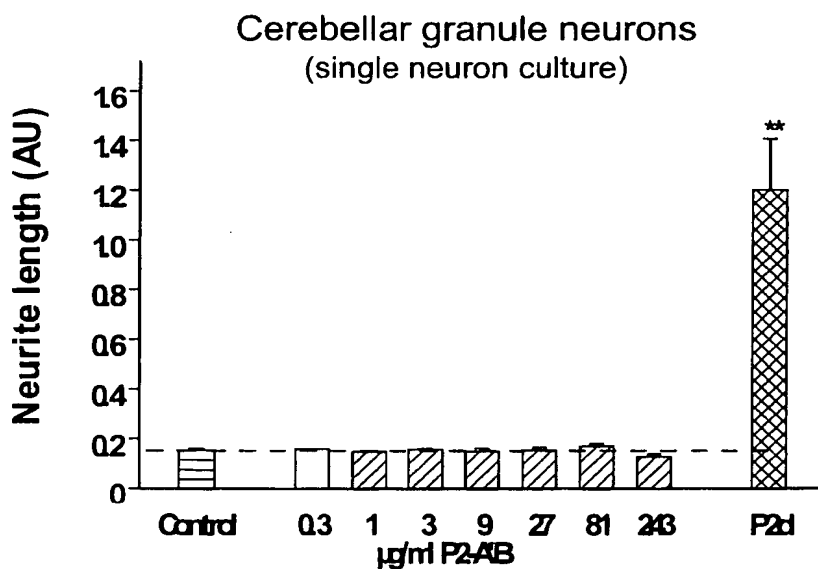
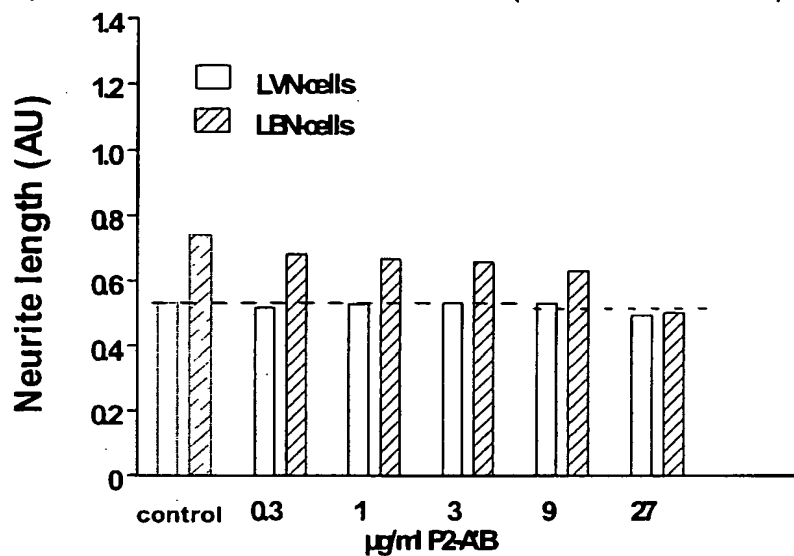


Figure 12